

# Nonequilibrium Statistical Mechanics and Hydrodynamics for a Granular Fluid

James W. Dufty

*Department of Physics, University of Florida, Gainesville, FL 32611*

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## Abstract

Granular fluids consist of collections of activated mesoscopic or macroscopic particles (e.g., powders or grains) whose flows often appear similar to those of normal fluids. To explore the qualitative and quantitative description of these flows an idealized model for such fluids, a system of smooth inelastic hard spheres, is considered. The single feature distinguishing granular and normal fluids being explored in this way is the inelasticity of collisions. The dominant differences observed in real granular fluids are indeed captured by this feature. Following a brief introductory description of real granular fluids and motivation for the idealized model, the elements of nonequilibrium statistical mechanics are recalled (observables, states, and their dynamics). Peculiarities of the hard sphere interactions are developed in detail. The exact microscopic balance equations for the number, energy, and momentum densities are derived and their averages described as the origin for a possible macroscopic continuum mechanics description. This formally exact analysis leads to closed, macroscopic hydrodynamic equations through the notion of a “normal” state. This concept is introduced and the Navier-Stokes constitutive equations are derived, with associated Green-Kubo expressions for the transport coefficients. A parallel description of granular gases is described in the context of kinetic theory, and the Boltzmann limit is identified critically. The construction of the “normal” solution to the kinetic equation is outlined, and Navier-Stokes order hydrodynamic equations are re-derived for a low density granular gas.

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## I. INTRODUCTION

Granular fluids are ubiquitous in nature [1, 2]. To illustrate with the familiar first, go to your kitchen and take out the mustard seeds, pepper corns, salt, and rice. Put 100 grains of each in small jars and tumble these jars in various directions. The gravitational field induces temporary flows of groups of grains in each case. While the flows appear to be locally convective it is clear that each grain's motion is more complex due to interactions with other grains. This is qualitatively similar to macroscopic flows of normal fluids (those composed of atoms or molecules) in which the coarse grained convection is the collective effect of complex atomic collisional motion. The objective here is to explore to what extent the well developed methods to describe the macroscopic dynamics of normal fluids [3] can be extended to the flow of such compositions of grains [4]. Clearly, there are significant differences in the physical systems. It will be seen that many properties of interest are insensitive to some of the most obvious differences, and that others can be incorporated in realistic models for the system of grains.

Normal fluids incorporate a wide range of different systems. Simple atomic fluids are well represented by spherically symmetric central point forces between the atomic constituents, and Navier-Stokes hydrodynamics (defined precisely below) applies to most macroscopic nonequilibrium states of interest in this case. The interactions in low molecular weight fluids no longer have spherical symmetry, but at the macroscopic level this is a quantitative rather than a qualitative effect (e.g., only the values of transport coefficients in the Navier-Stokes description change). Mixtures of these types of fluids also have the same qualitative macroscopic behavior. On the other hand complex fluids, such as those composed of high molecular weight (polymers), generally exhibit quite different macroscopic behavior which can depend on both the system and the class of macroscopic states considered.

Some of this diversity is evident for systems of grains as well. The mustard seeds are more mono disperse and smooth than the pepper corns, but both are roughly spherical. On the other hand rice is asymmetric to differing extents (e.g., large aspect ratio in China, small in Spain). As with normal fluids, their macroscopic flows are quite similar. Salt has irregular shape and furthermore is complicated by being hydrophilic - any moisture in the air changes dramatically the interaction between grains. This can change its motion as well, as everyone knows about salt shakers at the seaside. Thus, the medium in which the grains

move can be important. Structurally complex grains such as collections of filaments will not be considered here. Still, structurally simple granular systems can behave as complex fluids in many nonequilibrium states of interest. This is an important difference between normal fluids and granular systems that provides some of the most difficult challenges and also some of the most interesting opportunities.

Beyond the kitchen, granular systems include objects of interest to the pharmaceutical industry (pills and associated powders generated in their production), the agricultural industry (storage and transport of edible grains), geology (rock and snow avalanches), and extra-terrestrial systems (Saturn's rings, regolith on Mars). Two general classes of states for these granular systems are distinguished, *compact* and *activated*. Unshaken, the rice in the jar appears at rest. In fact, each grain has some kinetic energy due to the temperature of the room. However, on Earth the gravitational potential energy relative to the bottom of the container for heights  $h$  greater than the dimension of the grain is much larger than this energy of motion, due to the large mass of typical grains. Thus, they pack at the bottom of the container. Questions about the possible distribution of packing configurations constitutes a field of current activity [5], and is of central practical interest for the storage of grains. For example, granular storage in silos commonly leads to explosions whose mitigation requires knowledge of the distribution of forces in the packed grains. Here, attention is limited to the second class of *activated* grains. Work is done on the system (e.g., shaking) to provide a kinetic energy greater than that required to overcome the compactification by gravity. In addition, when the number of grains is large the activation typically induces an apparent random component to the granular motion due to frequent collisions among the grains. Systems of activated, collisional grains constitute the qualitative definition of *granular fluids* for the discussion here.

Phenomenologically, Navier-Stokes hydrodynamics has been applied to a wide class of granular flows in practice with qualitative success in many cases. To what extent can such a description be justified from a more fundamental basis? If justified, how can the parameters of this description (equation of state, energy loss function, transport coefficients) be given fundamental definitions as functions of the state conditions? If justified, what is the context and limitations of this description? These are the issues that are addressed here. As with the history of progress on these same questions for normal fluids, initial attention is focused on an idealized fluid and states where conceptual problems can be isolated and addressed

cleanly. Steps to describe more realistic granular fluids can then proceed with increased confidence and guidance. In the next section this idealized granular fluid is defined and the overview of its exploration is summarized.

## II. OVERVIEW OF THE PRESENTATION

The mustard seeds are hard, spherical, and monodisperse. This system can be refined for experiments using carefully machined spheres of glass or metal with empirically determined binary collision properties. Although hard, the binary collisions are quite complex in detail since each is composed of a large number of composite molecules. While in contact, the shape of each grain is distorted and energy is redistributed between the kinetic energy of their centers of mass and that of their internal degrees of freedom. On separation, they again move freely but with some energy lost to internal and rotational degrees of freedom. The "hard" interaction means that the contact time is short, so effectively the motion is that of free streaming punctuated by velocity changes on collision with a consequent loss of energy in each case. This suggests the idealization of a system of hard spheres (zero collision time) with inelastic collisions. A further simplification is the neglect of transfer between kinetic and rotational motion. This idealized fluid then consists of a system of smooth, inelastic hard spheres. It is similar to the idealized hard sphere fluid for normal atomic systems, with the sole difference being an energy loss on pair collisions.

In the next section the context of this ideal granular fluid is elaborated further to clarify the extent to which its properties should represent both qualitatively and quantitatively many properties of real granular fluids. The elements of nonequilibrium statistical mechanics are recalled briefly and applied to this system of hard, inelastic, smooth spheres [6, 7, 8]. Since the forces are singular, the usual form for the generator of dynamics for piecewise continuous forces no longer applies and the necessary changes are described in Appendix A. As a consequence of these changes the generators in different representations for the time dependence are different (e.g., that for the Liouville equation and that for the observables). Three different generators are identified in Appendix A. The average energy for an isolated system is shown to decrease monotonically due to the loss of energy on each binary collision. Consequently, there is no equilibrium Gibbs solution to the Liouville equation. Instead, it supports a "homogeneous cooling state" (HCS) in which the dynamics of the energy

loss appears only through a scaling of the velocities (hence the terminology "cooling") and associated normalization factors. Empirically (i.e., in molecular dynamics simulations) it is found that a wide class of homogeneous states approach the HCS after a few collisions per particle [9]. Consequently, the rapid velocity relaxation in normal fluids leading to the Gibbs distribution has its counterpart in this granular fluid in the approach on a similar time scale to the HCS distribution. The scaling form of the HCS suggests a related dimensionless representation for the Liouville equation in a more general context.

As described above, a main target of this investigation is the possibility of a macroscopic hydrodynamics. This refers to closed equations for the hydrodynamic observables: number density, energy density, and momentum density. As a fundamental starting point, the exact microscopic phase functions corresponding to these fields are identified and the balance equations for them are obtained in Appendix B. For a normal fluid, these are the local microscopic conservation laws. Section IV discusses the average of these equations, the macroscopic balance equations, which is the framework in which the corresponding hydrodynamic equations can exist. Contributions to the fluxes in these equations due to convection are identified from a local Galilean transformation [10]. The remaining contributions are due to "dissipative" exchanges of density, energy, and momentum for fluid cell at rest. The derivation of explicit expressions for this remainder, called "constitutive equations", is the central problem for obtaining hydrodynamic equations. A change of variables from density, energy density, and momentum density to density, temperature, and flow velocity is defined and introduced. Finally, the macroscopic state corresponding to the HCS is identified from these equations.

A more precise definition of hydrodynamics is considered in Section V, where the notion of "normal" states is introduced and motivated. It is shown how this concept leads to constitutive equations which are functionals of the hydrodynamic fields, giving in principle a set of five closed equations for the determination of these fields. The special case of weakly inhomogeneous states is considered in Section VI as an example, leading to the phenomenological Navier-Stokes equations for a granular fluid. Two important differences between normal and granular fluids are noted, long wavelength instability and the existence of new stationary states.

The formal construction of a normal solution to the Liouville equation is considered in Section VII for weakly inhomogeneous states by an expansion in the local spatial gradients.

The leading order reference state is a local HCS distribution, similar to the local equilibrium Gibbs distribution for normal fluids. The constitutive equations at this approximation provide definitions for the hydrostatic pressure and the local cooling rate in each fluid cell. The formal solution to the Liouville equation including first order in the gradients provides constitutive equations characterized by the transport coefficients for a granular fluids. This extends recent results obtained from a solution to the Liouville equation for small initial perturbations (linear response) [11, 12]. Expressions for these transport coefficients, the Green-Kubo formulas for granular fluids, also are discussed in Section VII. The specific case of shear viscosity is explored further for illustration. The simplest test of these formal developments is provided by the dynamics of a single impurity in a granular fluid in its HCS, corresponding to impurity motion in an equilibrium fluid. The expected hydrodynamics in this case is simple diffusion of the particle's probability density. The Green-Kubo expression for the diffusion coefficient is noted, and a practical short time approximation for the associated velocity autocorrelation function is demonstrated [13].

A different approach to the determination of constitutive equations is provided by kinetic theory, a representation in terms of the reduced single particle distribution function. This approach is described in Section VIII where the objects of interest are shown to be determined exactly by the single particle distribution function, and the hierarchy of equations determining all reduced distribution functions is derived from the Liouville equation. A formal solution to the hierarchy is obtained systematically at low density, resulting in a Boltzmann description for a granular gas. The derivation of hydrodynamics from this kinetic theory is outlined and compared to the general fluid results.

Finally, some additional perspective on these results is given in the Discussion Section. The analysis here suggests that hydrodynamics is a useful concept for granular fluids, but its context and limitations have not been explored in any detail. Appropriate space and time scales for hydrodynamics in general and limitations of the Navier-Stokes approximation in particular are discussed.

As these notes are prepared for a series of lectures the material is focused on the research of the author and his colleagues. The references quoted are heavily weighted in that direction as well. Apologies are offered at the outset for the many excellent contributions to this subject matter not given explicit recognition.

### III. IDEALIZED GRANULAR FLUID AND STATISTICAL MECHANICS

#### A. Hard sphere idealization

Consider a fluid comprised of mono-disperse, spherical particles with pairwise additive central interactions (i.e., smooth particles with no tangential momentum transfer). Also, assume that Newton's third law holds so that momentum is conserved between colliding pairs. More general cases of mixtures, non-central, or many-body forces can be incorporated with greater complexity but no significant conceptual changes. The case of dissipative "soft" spheres is considered first. The pair force is assumed to be piecewise continuous for relative distance between particles  $r$  and  $s$ ,  $q_{rs} \equiv |\mathbf{q}_r - \mathbf{q}_s| \leq \sigma$  and vanishing for  $q_{rs} > \sigma$ . As a central force it is directed along the line of centers  $\hat{\mathbf{q}}_{rs}$  and therefore has the form

$$\mathbf{F}(\mathbf{q}_{rs}, \mathbf{g}_{rs}) = \hat{\mathbf{q}}_{rs} \Theta(\sigma - q_{rs}) f(q_{rs}, g_{rs}, \hat{\mathbf{q}}_{rs} \cdot \hat{\mathbf{g}}_{rs}). \quad (3.1)$$

Here  $\mathbf{g}_{rs} = \mathbf{v}_r - \mathbf{v}_s$  is the velocity of approach or separation. From spherical symmetry the magnitude of the force can depend only on the scalars  $q_{rs}, g_{rs}, \hat{\mathbf{q}}_{rs} \cdot \hat{\mathbf{g}}_{rs}$ . The functional form of this force is such as to describe the two physical effects of repulsion and dissipation during the deformation. For example, it could be the superposition of an conservative repulsive elastic force plus a drag force proportional to the normal component of the relative velocity. The amount of deformation is then  $d \sim \sqrt{e/k}$  where  $e$  is the energy per particle and  $k$  is the elastic constant. The conditions of interest here are such that  $d/\sigma \ll 1$  and  $\tau_c/\tau_m \ll 1$ , where  $\tau_c \sim d\sqrt{m/e}$  is the average contact time and  $\tau_m \sim n^{-1/3}\sqrt{m/e}$  is the mean free time between collisions. Consequently,  $(\tau_c/\tau_m) \sim (n\sigma^3)^{1/3} (d/\sigma) < (d/\sigma)$  since  $n\sigma^3 < 1$  for fluid states. These are rough estimates, but they show that the controllable parameters  $e$  and  $k$  admit conditions where the particles behave as hard objects. A force law  $f(q_{rs}) \sim (\sigma/r)^n$  describes well the repulsive forces for simple atomic fluids, with  $n > 12$ , and its properties are known to be accurately represented by those for hard spheres  $n \rightarrow \infty$  [3]. A similar limit for the conservative part of the deformation potential can be expected as well.

It is necessary also to retain the fact that there is a total energy loss during the contact time in this hard sphere limit. This is done by requiring that the collisions are inelastic. In detail, the total momentum for the colliding pair is conserved and the relative velocity changes according to

$$\mathbf{g}'_{rs} = \mathbf{g}_{rs} - (1 + \alpha (\hat{\mathbf{q}}_{rs} \cdot \mathbf{g}_{rs})) (\hat{\mathbf{q}}_{rs} \cdot \mathbf{g}_{rs}) \hat{\boldsymbol{\sigma}}, \quad (3.2)$$

with the corresponding energy change

$$\Delta \left( \frac{1}{2} m (v_r^2 + v_s^2) \right) = \frac{1}{4} m (g_{rs}'^2 - g_{rs}^2) = -\frac{1}{4} m (1 - \alpha^2 (\hat{\mathbf{q}}_{rs} \cdot \mathbf{g}_{rs})) (\hat{\mathbf{q}}_{rs} \cdot \mathbf{g}_{rs})^2. \quad (3.3)$$

The scalar parameter  $\alpha (\hat{\mathbf{q}}_{rs} \cdot \mathbf{g}_{rs})$  is the restitution coefficient and takes on the values  $0 < \alpha \leq 1$ , with  $\alpha = 1$  corresponding to elastic collisions. A detailed correspondence between inelastic hard spheres and soft dissipative spheres requires that the restitution coefficient should depend on the normal component of the relative velocity [14]. In particular, it is found that  $\alpha (\hat{\mathbf{q}}_{rs} \cdot \mathbf{g}_{rs}) \rightarrow 1$  as  $\hat{\mathbf{q}}_{rs} \cdot \mathbf{g}_{rs} \rightarrow 0$ . However, if the conditions studied avoid this limit (e.g., continual energy input), then it is possible to consider the further idealization of an average energy loss per collision characterized by a constant restitution coefficient  $\alpha (\hat{\mathbf{q}}_{rs} \cdot \mathbf{g}_{rs}) \rightarrow \alpha$ . This will be the case studied in all of the following.

There is a mathematical price to be paid for this idealization of smooth, inelastic, hard spheres. The forces are singular at contact, and therefore the usual description of the dynamics from Hamilton's equations must be modified [10, 15, 16, 17]. The modification corresponds to replacing the effect of the continuous force by a binary scattering operator that generates the instantaneous momentum change of the pair on contact. The form of this operator is derived in Appendix A. This complication is common to the representation by hard spheres of both normal and granular fluids. In the latter case there is another, perhaps unexpected, effect of the hard collisions plus dissipation called inelastic collapse [18]. To understand this, consider a perfectly elastic hard ball dropped from a height  $h$  on a horizontal table in the gravitational field. Without interference it bounces indefinitely and it is never in contact with the table over any finite time interval. In contrast, the inelastic hard sphere will undergo an infinite number of collisions in a finite time  $\tau$  and come to rest in contact with the table. A similar effect occurs in the inelastic hard sphere granular fluid where groups of particles can cluster with increasing numbers of collisions among them in a finite time interval. The issue of inelastic collapse will be revisited at the end of this section.

## B. Overview of nonequilibrium statistical mechanics

For a given physical system its description via statistical mechanics consists of states (represented by distribution functions over its phase space), observables (phase space func-



tions), and expectation values (averages of the observables over the states). Its evolution in time is given by a mapping of either the states or the observables in phase space. The system of interest here is a one component fluid of  $N$  identical smooth, inelastic, hard spheres (mass  $m$ , diameter  $\sigma$ ). The state of the system at time  $t = 0$  is completely characterized by the positions and velocities of all particles, represented by a point in a  $6N$  dimensional phase space  $\Gamma_0 \equiv \{\mathbf{q}_1(0), \dots, \mathbf{q}_N(0), \mathbf{v}_1(0), \dots, \mathbf{v}_N(0)\}$ . The dynamics consists of straight line motion along the direction of the velocity at time  $t$  (free streaming), until any pair of particles, say  $i, j$ , is in contact. The relative velocity  $\mathbf{g}_{ij} = \mathbf{v}_i - \mathbf{v}_j$  of that pair changes instantaneously according to a given collision rule (3.2) while their total momentum is unchanged. Subsequently, all particles continue to stream freely until another pair is at contact, and the collisional change is repeated for that pair. In this way a unique trajectory  $\Gamma_t \equiv \{\mathbf{q}_1(t), \dots, \mathbf{q}_N(t), \mathbf{v}_1(t), \dots, \mathbf{v}_N(t)\}$  is generated in the phase space for  $t > 0$ , where the configurational degrees of freedom change continuously while those for the velocities are piecewise constants.

The statistical mechanics for a fluid of inelastic hard spheres has been described elsewhere [6, 7, 8, 19, 20]. It is comprised of the dynamics just described, a macrostate specified in terms of a probability density  $\rho(\Gamma)$ , and a set of observables denoted by  $A(\Gamma)$ . The expectation value for an observable at time  $t > 0$  for a state  $\rho(\Gamma)$  given at  $t = 0$  is defined by

$$\langle A(t); 0 \rangle \equiv \int d\Gamma \rho(\Gamma) A(\Gamma_t) \quad (3.4)$$

where  $A(t) = A(\Gamma_t)$ , and  $\Gamma_t \equiv \{\mathbf{q}_1(t), \dots, \mathbf{q}_N(t), \mathbf{v}_1(t), \dots, \mathbf{v}_N(t)\}$  is the phase point evolved to time  $t$  from  $\Gamma = \Gamma_{t=0}$ . The dynamics can be represented in terms of a generator  $L$  defined by

$$\langle A(t); 0 \rangle = \int d\Gamma \rho(\Gamma) e^{tL} A(\Gamma). \quad (3.5)$$

For continuous potentials the generator is easily recognized from Hamilton's equation as a Poisson bracket operation with the corresponding Hamiltonian. However, its identification for the discontinuous hard sphere potential is less direct [10, 15, 16, 17]. There are two components to the generator, corresponding to the two steps of free streaming and velocity changes at contact. The first part is the same as for continuous potentials while the second part replaces the contribution from the singular force by a "binary collision operator"  $T(i, j)$

for each pair  $i, j$  [21]

$$L = \sum_{i=1}^N \mathbf{v}_i \cdot \nabla_i + \frac{1}{2} \sum_{i=1}^N \sum_{j \neq i}^N T(i, j). \quad (3.6)$$

The binary collision operator  $T(i, j)$  for normal fluids is identified directly from the Poisson bracket of Hamilton's equations

$$T(i, j) \rightarrow \theta_{ij} = m^{-1} \mathbf{F}(q_{ij}) \cdot (\nabla_{\mathbf{v}_i} - \nabla_{\mathbf{v}_j}). \quad (3.7)$$

where  $\mathbf{F}(q_{ij})$  is a conservative force. For hard spheres, the position variables are still continuous functions of time but the momenta are piecewise constant (in the absence of external forces) and discontinuous. The form for  $T(i, j)$  in this case is obtained in Appendix A with the result

$$T(i, j) = \Theta(-\mathbf{g}_{ij} \cdot \hat{\mathbf{q}}_{ij}) |\mathbf{g}_{ij} \cdot \hat{\mathbf{q}}_{ij}| \delta(q_{ij} - \sigma) (b_{ij} - 1), \quad (3.8)$$

where  $\Theta$  is the Heaviside step function, and  $b_{ij}$  is a substitution operator which changes the relative velocity  $\mathbf{g}_{ij}$  into its scattered value  $\mathbf{g}'_{ij}$ , given by Eq. (3.2)

$$b_{ij} A(\mathbf{g}_{ij}) = A(\mathbf{g}'_{ij}). \quad (3.9)$$

The theta function and delta function in (3.8) assure that a collision takes place, i.e. the pair is at contact and directed toward each other.

An alternative equivalent representation of the dynamics is obtained by transferring the dynamics from the observable  $A(\Gamma)$  to the state  $\rho(\Gamma)$  by the definition

$$\int d\Gamma \rho(\Gamma) e^{tL} A(\Gamma) \equiv \int d\Gamma \left( e^{-t\bar{L}} \rho(\Gamma) \right) A(\Gamma). \quad (3.10)$$

The representation in terms of a dynamical state is referred to as Liouville dynamics. The probability density  $\rho(\Gamma)$  must vanish for all configurations of overlapping hard spheres, so the domain of integration on the left side of (3.10) is effectively restricted to non-overlapping configurations. Thus the generator  $L$  is used always in that context. However, the right side of (3.10) no longer has that restriction and consequently the generator for Liouville dynamics is not the same as that for observables (as in the case of continuous potentials). Instead, direct analysis of (3.10) leads to the result (see Appendix A)

$$\bar{L} = \sum_{i=1}^N \mathbf{v}_i \cdot \nabla_i - \frac{1}{2} \sum_{i=1}^N \sum_{j \neq i}^N \bar{T}(i, j), \quad (3.11)$$

with the new binary collision operator

$$\overline{T}_-(i, j) = \delta(q_{ij} - \sigma) |\mathbf{g}_{ij} \cdot \hat{\mathbf{q}}_{ij}| (\Theta(\mathbf{g}_{ij} \cdot \hat{\mathbf{q}}_{ij}) \alpha^{-2} b_{ij}^{-1} - \Theta(-\mathbf{g}_{ij} \cdot \hat{\mathbf{q}}_{ij})). \quad (3.12)$$

Here  $b_{ij}^{-1}$  is the inverse of the operator  $b_{ij}$  in (3.9).

Next consider time correlation functions for two observables  $A$  and  $B$

$$\langle A(t)B; 0 \rangle \equiv \int d\Gamma (e^{tL} A(\Gamma)) \rho(\Gamma) B(\Gamma) = \int d\Gamma A(\Gamma) e^{-t\overline{L}} (\rho(\Gamma) B(\Gamma)). \quad (3.13)$$

A third generator is defined for reversed dynamics along the trajectory by

$$e^{-t\overline{L}} (\rho(\Gamma) B(\Gamma)) \equiv (e^{-t\overline{L}} \rho(\Gamma)) (e^{-tL_-} B(\Gamma)). \quad (3.14)$$

This gives

$$\begin{aligned} \langle A(t)B; 0 \rangle &= \int d\Gamma A(\Gamma) e^{-t\overline{L}} (\rho(\Gamma) B(\Gamma)) = \int d\Gamma \rho(\Gamma, t) A(\Gamma) e^{-tL_-} B(\Gamma) \\ &= \langle AB(-t); t \rangle. \end{aligned} \quad (3.15)$$

where the reversed dynamics of  $B(-t)$  has been defined by

$$B(-t) \equiv e^{-tL_-} B(\Gamma). \quad (3.16)$$

The new generator is identified in Appendix A as

$$L_- = \sum_{i=1}^N \mathbf{v}_i \cdot \nabla_{\mathbf{q}_i} - \frac{1}{2} \sum_{i=1}^N \sum_{j \neq i}^N T_-(i, j) \quad (3.17)$$

with

$$T_-(i, j) = \delta(q_{ij} - \sigma) \Theta(\hat{\mathbf{g}}_{ij} \cdot \hat{\mathbf{q}}_{ij}) |\mathbf{g}_{ij} \cdot \hat{\mathbf{q}}_{ij}| (b_{ij}^{-1} - 1) \quad (3.18)$$

In summary, the problems presented by the singular forces for a fluid of hard spheres are resolved if Hamilton's equations for observables are replaced by

$$(\partial_t - L) A(\Gamma, t) = 0, \quad (\partial_t + L_-) A(\Gamma, -t) = 0 \quad (3.19)$$

and the Liouville equation for probability densities is replaced by

$$(\partial_t + \overline{L}) \rho(\Gamma, t) = 0, \quad (3.20)$$

for  $t \geq 0$ , with the respective generators given by (3.6), (3.17), and (3.11). The three generators are all different, so some care must be used to apply them under the correct conditions

of their definitions. Note that the forms of the generators  $L$  and  $L_-$ , and corresponding binary collision operators  $T(i, j)$  and  $T_-(i, j)$ , do not depend on the details of the collision rule defining the operator  $b_{ij}$ ; the result applies for both elastic and inelastic collisions [21]. In contrast, the generator for Liouville dynamics is obtained by a change of variables that introduces the Jacobian of the transformation between the variables  $\mathbf{g}_{ij}$  and  $b_{ij}\mathbf{g}_{ij}$ . Hence it depends explicitly on the collision rule and the restitution coefficient  $\alpha$ .

For normal fluids the probability of a configuration with any pair of particles in contact and at rest has vanishing measure. Then the above description of trajectories as sequences of pair collisions among the particles is adequate. As noted above, in granular fluids the phenomenon of inelastic collapse admits the possibility of evolution to a state where clusters of particles are in contact and at rest. It would appear that the collision of another particle with that cluster be described would require a more complex generator for the dynamics than that considered here. Consider the simplest case of a pair in contact and at rest, with a third particle incident on one of the two. The generator here would transfer momentum to one of the pair, as though it were isolated. Then, it would no longer be at rest with respect to the other member of the pair and a second instantaneous momentum transfer would occur to the second member. As a result, both particles originally at contact and in relative rest would experience relative motion and all three particles would separate. In fact, this is the correct dynamics for real particles and it avoids the difficulty of indeterminate dynamics for collisions with clusters. Mathematically, therefore, there appears to be no difficulty for the dynamics generated here due to inelastic collapses. In practice, however, this can be difficult to simulate as the effective time between such collisions can be very small and require following a large number of collisions.

### C. Homogeneous cooling state

In the absence of external forces there is special solution to the Liouville equation for normal fluids: the stationary, homogenous (translationally invariant) equilibrium solution,  $\rho_e$ . For the isolated system considered here this is a probability density with sharply defined total energy, total momentum, and number of particles. It is “universal” in the sense that most other homogeneous initial preparations rapidly approach this stationary equilibrium solution, on a time scale of the order of several collisions per particle. This is the collisional

velocity relaxation to Maxwellian distributions for each velocity degree of freedom. Granular fluids are different in the sense that the Liouville equation for an isolated system has no stationary solution. This is due to the loss of energy on each inelastic collision, such that the total energy decreases monotonically  $E(t) < E(0)$ . Nevertheless, it appears there is a universal homogeneous solution  $\rho_h$  whose time dependence occurs entirely through a scaling of the velocities for each particle [22]

$$\rho_h(\Gamma; t) = (lv_h(t))^{-Nd} \rho_h^* \left( \left\{ \frac{\mathbf{q}_{rs}}{l}, \frac{\mathbf{v}_r - \mathbf{U}_h}{v_h(t)} \right\} \right). \quad (3.21)$$

Here  $\mathbf{q}_{rs} = \mathbf{q}_r - \mathbf{q}_s$ , and  $\mathbf{U}_h$  is an overall constant velocity of the system. This velocity can be removed by a Galilean transformation but it is useful to retain it for the generalization to a corresponding local form defined below. Also,  $l$  is an arbitrary constant characteristic length and  $v_h(t)$  is a "thermal" velocity defined in terms of the energy per particle

$$v_h^2(t) = \frac{2T_h(t)}{m}, \quad T_h(t) \equiv \frac{2E_h(t)}{3N} = \frac{2}{3N} \int d\Gamma \left( \sum_r \frac{1}{2} m v_r^2 \right) \rho_h(\Gamma; t) \quad (3.22)$$

The second equality defines an associated "temperature" for the system, so that  $v_h(t)$  can be interpreted as the average thermal speed. This temperature definition agrees with that introduced below for one of the hydrodynamic fields. Then,  $\rho_h(\Gamma; t) = \rho_h(\Gamma; T(t))$  is an example of a "normal" state, also defined below, whose time dependence occurs entirely through the hydrodynamic fields.

The specific form for  $\rho_h^*$  is determined by the requirement that  $\rho_h$  should be a solution to the Liouville equation (3.20)

$$(\partial_t T_h) \partial_{T_h} \rho_h + \bar{\mathcal{L}} \rho_h = 0, \quad (3.23)$$

or

$$\bar{\mathcal{L}}_{T_h} \rho_h = 0, \quad \bar{\mathcal{L}}_T = -\zeta_h(T) T \partial_T + \bar{\mathcal{L}} \quad (3.24)$$

The "cooling rate"  $\zeta_h$  has been introduced by the definition

$$\zeta_h(T_h(t)) \equiv -T_h^{-1}(t) \partial_t T_h(t). \quad (3.25)$$

The scaling property (3.21) gives an equivalent alternative form

$$\bar{\mathcal{L}} \rho_h = 0, \quad (3.26)$$

where the operator  $\bar{\mathcal{L}}$  is defined by

$$\bar{\mathcal{L}}X = \frac{\zeta_h}{2} \sum_{r=1}^N \nabla_{\mathbf{v}_r} \cdot [(\mathbf{v}_r - \mathbf{U}_h) X] + \bar{L}X. \quad (3.27)$$

An explicit expression for the cooling rate in terms of  $\rho_h$  follows from differentiation of (3.22) with respect to time and using the Liouville equation to get

$$\begin{aligned} \zeta_h &= \frac{1}{T_h N} \int d\Gamma \left( \sum_r \frac{1}{3} m v_r^2 \right) \bar{L} \rho_h(\Gamma; t) \\ &= -\frac{1}{T_h N} \int d\Gamma \left( L \sum_r \frac{1}{3} m v_r^2 \right) \rho_h(\Gamma; t) \\ &= -(N-1) \frac{m}{6T_h(t)} \int d\Gamma \rho_h(\Gamma; t) T(i, j) (v_i^2 + v_j^2). \end{aligned} \quad (3.28)$$

Recalling the explicit form for  $T(i, j)$  in (3.8), the cooling rate is seen to be proportional to the energy changes on binary collisions given by (3.3). The cooling rate then simplifies to

$$\zeta_h = (1 - \alpha^2) \frac{Nm}{12T_h(t)} \int d\Gamma \rho_h(\Gamma, t) (\mathbf{g}_{12} \cdot \hat{\mathbf{q}}_{12})^3 \Theta(\mathbf{g}_{12} \cdot \hat{\mathbf{q}}_{12}) \delta(q_{12} - \sigma). \quad (3.29)$$

Note that since  $\rho_h(\Gamma; t)$  depends on time only through  $T_h(t)$  the cooling rate also has this property, as the notation in (3.25) implies.

In summary, the special HCS solution to the Liouville equation  $\rho_h(\Gamma; t)$  is defined by (3.26) together with (3.29) which is a linear functional of  $\rho_h(\Gamma; t)$ . In this representation, the linear Liouville equation in terms of  $\Gamma, t$  becomes a nonlinear equation parameterized by  $T_h(t)$ . In principle, the solution is determined in two steps. First, (3.26) and (3.29) are solved as a function of  $T_h(t)$ . Second  $T_h(t)$  is determined from (3.25) and substituted into the solution found in the first step. The time dependence from this second step can be determined quite generally from the scaling property of his dependence on  $T_h(t)$  can be made explicit through the scaling form of (3.21) which leads to

$$\zeta_h(T_h(t)) = \frac{v_h(t)}{\ell} \zeta_h^*, \quad (3.30)$$

where  $\zeta_h^*$  is a constant

$$\zeta_h^* = (1 - \alpha^2) \frac{N}{6} \int d\Gamma^* \rho_h^*(\Gamma^*) (\mathbf{g}_{12}^* \cdot \hat{\mathbf{q}}_{12})^3 \Theta(\mathbf{g}_{12}^* \cdot \hat{\mathbf{q}}_{12}) \delta(q_{12}^* - \frac{\sigma}{\ell}). \quad (3.31)$$

The dimensionless variables for the integration here are given by

$$\Gamma^* \equiv \{\mathbf{q}_1^*, \dots, \mathbf{q}_N^*, \mathbf{v}_1^* \dots, \mathbf{v}_N^*\}, \quad \mathbf{q}_r^* = \frac{\mathbf{q}_r}{l}, \quad \mathbf{v}_r^* = \frac{\mathbf{v}_r - \mathbf{U}_h}{v_h(t)}. \quad (3.32)$$

Thus (3.30) exposes the explicit temperature dependence of  $\zeta_h(T_h(t))$  and (3.25) becomes

$$\partial_t T_h^{-1/2}(t) = \frac{\zeta_h^*}{\ell\sqrt{2m}}, \quad (3.33)$$

which can be integrated to give [4]

$$T_h(t) = T_h(0) \left( 1 + \frac{v_h(0)\zeta_h^*}{2\ell} t \right)^{-2} \rightarrow \ell^2 m \zeta_h^{*-2} t^{-2}. \quad (3.34)$$

The initial time has been chosen at  $t = 0$  without loss of generality. The long time cooling is seen to be algebraic and universal (independent of initial conditions). Thus,  $\rho_h(\Gamma; t)$  is a universal function of  $T_h(t)$  which itself becomes universal at long times.

#### D. Dimensionless representations

These last considerations suggest that the mathematics may be simpler and the physics better exposed by using a representation in terms of the dimensionless variables (3.32) [12, 19, 20]. The associated dimensionless time is defined through the differential form

$$ds = \frac{v_h(t)}{\ell} dt. \quad (3.35)$$

This can be integrated using (3.34) to give

$$s(t, 0) = \frac{2}{\zeta_h^*} \ln \left( \frac{v_h(0)\zeta_h^*}{2\ell} t \right). \quad (3.36)$$

The parameter  $s(t, 0)$  is a measure of the average number of collisions per particle in the interval  $(0, t)$ . In terms of this parameter the cooling of (3.34) becomes exponential

$$\frac{T_h(t)}{T_h(0)} = e^{-\zeta_h^* s}. \quad (3.37)$$

The dimensionless form of (3.26) is

$$\overline{\mathcal{L}}^* \rho_h^* = 0, \quad (3.38)$$

with

$$\overline{\mathcal{L}}^* X = \frac{\zeta_h^*}{2} \sum_{r=1}^N \nabla_{\mathbf{v}_r^*} \cdot [\mathbf{v}_r^* X] + \overline{L}^* X. \quad (3.39)$$

This equation is supplemented by the definition of  $\zeta_h^*$  in terms of  $\rho_h^*$  in (3.31). There is no longer any time dependence, no dependence on  $T_h(t)$ , only a parameterization of the solution by the scalar  $\zeta_h^*$ . Further elaboration on this is given below.

Now return to the more general solutions to the Liouville equation given by (3.20). Each solution will be characterized by an initial total energy, momentum, and particle number. For these global parameters there is an associated  $\rho_h$  and  $T_h(t)$  defined. The equation for general solutions can be expressed in terms of the same dimensionless variables (3.32) and (3.35) for the associated HCS. The result is [20]

$$\left(\partial_s + \overline{\mathcal{L}}^*\right) \rho^* = 0, \quad \rho(\Gamma; t) = (lv_h(t))^{-Nd} \rho^*(\Gamma^*; s). \quad (3.40)$$

The dimensionless generator for the dynamics,  $\overline{\mathcal{L}}^*$ , is the same as that given in (3.39). This result is similar in form to the original representation of the Liouville equation, except that now the time is measured in terms of the average number of collisions and the generator for the dynamics has an additional contribution compensating for collisional cooling as it would occur in the corresponding HCS. Note that in this representation  $\rho_h^*$  is a stationary solution to the Liouville equation (3.40). The differences between normal and granular fluids have been somewhat mitigated by this dimensionless representation. For example, notions of "approach to equilibrium" can be translated into "approach to the HCS", and the universal features of the equilibrium state can be translated to those of the HCS. MD simulations suggest that these comparisons are useful in the sense that very different homogeneous initial conditions approach the HCS on a time scale of several collisions per particle [9]. The corresponding dimensionless representations for observables corresponding to (3.19) are

$$(\partial_s - \mathcal{L}^*) A^*(\Gamma^*; s) = 0, \quad (\partial_s + \mathcal{L}_-^*) A^*(\Gamma^*; -s) = 0, \quad (3.41)$$

$$\mathcal{L}^* X = -\frac{\zeta_h^*}{2} \sum_{r=1}^N \mathbf{v}_r^* \cdot \nabla_{\mathbf{v}_r^*} X + L^* X, \quad \mathcal{L}_-^* X = \frac{\zeta_h^*}{2} \sum_{r=1}^N \mathbf{v}_r^* \cdot \nabla_{\mathbf{v}_r^*} X + L_-^* X \quad (3.42)$$

#### IV. MACROSCOPIC BALANCE EQUATIONS

For a simple one component fluid the relevant macroscopic variables are the average number density  $n$ , energy density  $e$ , and momentum density  $\mathbf{g}$

$$n(\mathbf{r}, t) = \langle \hat{n}(\mathbf{r}); t \rangle, \quad e(\mathbf{r}, t) = \langle \hat{e}(\mathbf{r}); t \rangle, \quad \mathbf{g}(\mathbf{r}, t) = \langle \hat{\mathbf{g}}(\mathbf{r}); t \rangle. \quad (4.1)$$

The brackets denotes an average over the ensemble  $\rho(\Gamma, t)$  as indicated on the right side of (3.14)

$$\langle X; t \rangle \equiv \int d\Gamma \left( e^{-t\overline{L}} \rho(\Gamma) \right) X(\Gamma). \quad (4.2)$$



This set will be referred to as the hydrodynamic fields, as it is their macroscopic dynamics which is the candidate for a closed description on some appropriate length and time scale. The specific forms of the phase functions are given in Appendix B (a caret has been introduced to distinguish the microscopic and macroscopic fields). Also in that Appendix the exact microscopic balance equations for the phase functions are derived. Their averages give the corresponding macroscopic balance equations

$$\partial_t n(\mathbf{r}, t) + m^{-1} \nabla_{\mathbf{r}} \cdot \mathbf{g}(\mathbf{r}, t) = 0 \quad (4.3)$$

$$\partial_t e(\mathbf{r}, t) + \nabla_{\mathbf{r}} \cdot \langle \mathbf{s}(\mathbf{r}); t \rangle = \langle w(\mathbf{r}); t \rangle \quad (4.4)$$

$$\partial_t g_{\alpha}(\mathbf{r}, t) + \nabla_{\mathbf{r}_{\beta}} \langle h_{\alpha\beta}(\mathbf{r}); t \rangle = 0. \quad (4.5)$$

Here  $\langle \mathbf{s}(\mathbf{r}, t); 0 \rangle$  is the average energy flux,  $\langle w(\mathbf{r}, t); 0 \rangle$  is the average energy loss function, and  $\langle h_{\alpha\beta}(\mathbf{r}, t); 0 \rangle$  is the average momentum flux. Again, the phase functions  $\mathbf{s}(\mathbf{r}, t)$ ,  $w(\mathbf{r}, t)$ , and  $h_{\alpha\beta}(\mathbf{r}, t)$  are given explicitly in Appendix B [12]. These exact equations are the starting point for investigating the possibility of a hydrodynamic description for a granular fluid.

To further simplify the balance equations it is useful to define the average flow velocity according to

$$\mathbf{g}(\mathbf{r}, t) \equiv n(\mathbf{r}, t) m \mathbf{U}(\mathbf{r}, t). \quad (4.6)$$

Then as shown in Appendix C the purely convective parts of the energy and fluxes can be extracted by a local Galilean transformation [10]

$$e(\mathbf{r}, t) = e'(\mathbf{r}, t) + \frac{1}{2} m n(\mathbf{r}, t) U^2(\mathbf{r}, t) \quad (4.7)$$

$$\langle s_{\alpha}(\mathbf{r}); t \rangle = \langle s'_{\alpha}(\mathbf{r}); t \rangle + U_{\alpha}(\mathbf{r}, t) \left( e'(\mathbf{r}, t) + \frac{1}{2} m n(\mathbf{r}, t) U^2(\mathbf{r}, t) \right) + \langle h'_{\alpha\beta}(\mathbf{r}); t \rangle U_{\beta}(\mathbf{r}, t) \quad (4.8)$$

$$\langle h_{\alpha\beta}(\mathbf{r}); t \rangle = \langle h'_{\alpha\beta}(\mathbf{r}); t \rangle + m n(\mathbf{r}, t) U_{\alpha}(\mathbf{r}, t) U_{\beta}(\mathbf{r}, t) \quad (4.9)$$

The phase functions with a prime denote the same function evaluated at  $\mathbf{v}_i \rightarrow \mathbf{v}'_i = \mathbf{v}_i - \mathbf{U}(\mathbf{r}, t)$ . Therefore,  $e'(\mathbf{r}, t)$  is the rest frame "thermal energy",  $\langle \mathbf{s}'(\mathbf{r}); t \rangle$  is the rest frame "heat flux", and  $\langle h'_{\alpha\beta}(\mathbf{r}); t \rangle$  is the rest frame "pressure tensor". This terminology does not imply any thermodynamic implications, however, and it is useful to retain the names for comparison with normal fluid forms. In this spirit, the following notation is introduced

$$e'(\mathbf{r}, t) \equiv \frac{3}{2} n(\mathbf{r}, t) T(\mathbf{r}, t), \quad \zeta(\mathbf{r}, t) \equiv -\frac{2}{3 n(\mathbf{r}, t) T(\mathbf{r}, t)} \langle w(\mathbf{r}); t \rangle, \quad (4.10)$$

$$\langle \mathbf{s}'(\mathbf{r}); t \rangle \equiv \mathbf{q}(\mathbf{r}, t), \quad \langle h'_{\alpha\beta}(\mathbf{r}); t \rangle \equiv P_{\alpha\beta}(\mathbf{r}, t) \quad (4.11)$$

Equation (4.10) defines the "granular temperature". As a definition,  $T(\mathbf{r}, t)$  is meaningful for any state of the system as a measure of the local kinetic energy  $e'(\mathbf{r}, t)$  - it simply constitutes a change of variables from the pair  $(n, e', \mathbf{U})$  to  $(n, T, \mathbf{U})$  as the hydrodynamic fields of interest. However, its relationship to any given measuring device ("thermometer") must be considered with care. Similarly, (4.11) gives a microscopic definition for the heat flux  $\mathbf{q}(\mathbf{r}, t)$  and pressure tensor  $P_{\alpha\beta}(\mathbf{r}, t)$ . The interpretation of  $\zeta(\mathbf{r}, t)$  as a "cooling rate" appears in (4.13) directly below.

In terms of these new variables the macroscopic balance equations become

$$D_t n(\mathbf{r}, t) + n(\mathbf{r}, t) \nabla_{\mathbf{r}} \cdot \mathbf{U}(\mathbf{r}, t) = 0 \quad (4.12)$$

$$(D_t + \zeta(\mathbf{r}, t)) T(\mathbf{r}, t) + \frac{2}{3n(\mathbf{r}, t)} (P_{\alpha\beta}(\mathbf{r}, t) \partial_{\alpha} U_{\beta}(\mathbf{r}, t) + \nabla \cdot \mathbf{q}(\mathbf{r}, t)) = 0, \quad (4.13)$$

$$D_t U_{\alpha}(\mathbf{r}, t) + (mn(\mathbf{r}, t))^{-1} \partial_{\beta} P_{\alpha\beta}(\mathbf{r}, t) = 0, \quad (4.14)$$

where  $D_t = \partial_t + \mathbf{U} \cdot \nabla$  is the material derivative. These macroscopic balance equations are still exact. They have the same form as for a normal fluid, with the only change being the presence of the cooling rate. These are not a closed set of equations for  $n$ ,  $T$ , and  $\mathbf{U}$  since the heat flux, pressure tensor, and cooling rate have not been explicitly represented. Clearly, however, at this point these equations apply equally well to both granular and normal fluids under the most general fluid state conditions.

## V. "NORMAL" STATES, CONSTITUTIVE RELATIONS, AND HYDRODYNAMICS

The most general notion of a hydrodynamic description is a closed set of equations for the hydrodynamic fields,  $\{y_{\alpha}\} \Leftrightarrow \{n, T, \mathbf{U}\}$ . This follows from the exact macroscopic balance equations if the cooling rate, heat flux, and pressure tensor can be represented as functionals of these fields

$$\zeta(\mathbf{r}, t) \rightarrow \zeta(\mathbf{r}, t | \{y_{\alpha}\}), \quad \mathbf{q}(\mathbf{r}, t) \rightarrow \mathbf{q}(\mathbf{r}, t | \{y_{\alpha}\}), \quad P_{\alpha\beta}(\mathbf{r}, t) \rightarrow P_{\alpha\beta}(\mathbf{r}, t | \{y_{\alpha}\}) \quad (5.1)$$

These are known as constitutive relations. A comment on notation is appropriate at this point:  $f(\mathbf{r}, t, \{y_{\alpha}(\mathbf{r}, t)\})$  denotes a *function* of  $\mathbf{r}, t$  and the fields  $\{y_{\alpha}(\mathbf{r}, t)\}$  at the point  $\mathbf{r}$ ,

while  $f(\mathbf{r}, t | \{y_\alpha\})$  denotes a function of  $\mathbf{r}, t$  and a *functional* of  $\{y_\alpha\}$  at all space points. With such relations the macroscopic balance equations (4.12) - (4.14) become hydrodynamic equations, i.e.

$$\partial_t y_\alpha(\mathbf{r}, t) = N_\alpha(\mathbf{r}, t | \{y_\alpha\}). \quad (5.2)$$

The conditions for the existence of constitutive equations then constitute the context for a hydrodynamic description. Certainly, it cannot be expected in general that the fluxes can be characterized entirely by the hydrodynamic fields for all length and time scales. On the other hand important examples exist, such as the pressure tensor for an equilibrium fluid in an arbitrary external potential (density functional theory).

The connection of this question to the statistical mechanical basis for hydrodynamics follows from the fact that the cooling rate and fluxes are linear functionals of the solution to the Liouville equation, i.e. averages of the form (4.2). Therefore, a sufficient condition for constitutive equations is for the distribution function to be characterized by the hydrodynamic fields. A class of "normal" distributions is defined by the functional forms

$$\rho_n(\Gamma, t) = \rho_n(\Gamma | \{y_\alpha\}) \quad (5.3)$$

This means that all time dependence and all the breaking of translational invariance occurs only through the hydrodynamic fields. A familiar example of a normal distribution for real fluids is the local canonical distribution

$$\rho_{el}(\Gamma | \{y_\alpha\}) = \exp \left\{ q - \int d\mathbf{r} T^{-1}(\mathbf{r}, t) (\tilde{\mathcal{E}}'(\mathbf{r}) - \mu(\mathbf{r}, t) \hat{n}(\mathbf{r})) \right\} \quad (5.4)$$

where  $q$  is a normalization constant, and  $\mu(\mathbf{r}, t)$  is the chemical potential (as a specified function of the density and temperature for the hydrodynamic fields chosen here). If a normal solution to the Liouville can be found then the constitutive equations follow immediately

$$\zeta(\mathbf{r}, t | \{y_\alpha\}) = \frac{2}{3n(\mathbf{r}, t)T(\mathbf{r}, t)} \int d\Gamma \rho_n(\Gamma | \{y_\alpha\}) w(\mathbf{r}) \quad (5.5)$$

$$\mathbf{q}(\mathbf{r}, t | \{y_\alpha\}) = \int d\Gamma \rho_n(\Gamma | \{y_\alpha\}) \mathbf{s}'(\mathbf{r}) \quad (5.6)$$

$$P_{\alpha\beta}(\mathbf{r}, t | \{y_\alpha\}) = \int d\Gamma \rho_n(\Gamma | \{y_\alpha\}) h'_{\alpha\beta}(\mathbf{r}) \quad (5.7)$$

The origin of hydrodynamics has now been "reduced" to finding conditions for the existence of a normal solution to the Liouville equation. Its time derivative in the Liouville

equation can be expressed in terms of the hydrodynamic equations (5.2)

$$\partial_t \rho_n = \int d\mathbf{r} \frac{\delta \rho_n}{\delta y_\alpha(\mathbf{r}, t)} \partial_t y_\alpha(\mathbf{r}, t) = \int d\mathbf{r} \frac{\delta \rho_n}{\delta y_\alpha(\mathbf{r}, t)} N_\alpha(\mathbf{r}, t | \{y_\alpha\}).$$

Substitution of (5.3) into the Liouville equation gives the form for normal solutions

$$\int d\mathbf{r} \frac{\delta \rho_n}{\delta y_\alpha(\mathbf{r}, t)} N_\alpha(\mathbf{r}, t | \{y_\alpha\}) + \bar{L} \rho_n = 0. \quad (5.8)$$

This intimate connection of constructing a hydrodynamic description and finding a normal solution to the Liouville equation is in fact a single self-consistent problem. For specified fields, (5.8) is an equation for the  $\Gamma$  dependence of the normal phase space density as a function of the fields. This dependence then allows determination of the normal forms in (5.5) - (5.7). Finally, solution of the hydrodynamic equations (5.2), with suitable initial and boundary conditions, provides the explicit forms for the fields, and completes the normal solution. The existence and determination of this solution is the central problem for establishing a hydrodynamic description for both normal and granular fluids.

The concept of a normal solution and its use in the macroscopic balance equations makes no special reference to the possible inelasticity of collisions. Nor does the concept refer to states near homogeneity or the requirement of representation as local partial differential equations. As will be seen below, the familiar Navier-Stokes equations represent a special case of this more general idea. For normal fluids, the simple form of the Navier-Stokes equations applies for a wide range of structurally simple fluids, with rheology as a counter example for more complex fluids. As noted in the Introduction, even structurally simple granular fluids can exhibit behavior like complex real fluids for which the Navier-Stokes representation fails [23]. However, the generality of the discussion here shows that the failure of a Navier-Stokes approximation should not be taken as the absence of a more complex hydrodynamic description.

To clarify the conditions under which a normal solution could be expected, consider first a normal fluid with elastic collisions in an initial non-equilibrium state with specified hydrodynamic fields  $\{y_\alpha(\mathbf{r}, t = 0)\}$ , whose values vary smoothly across the system. In each small cell the phase space density  $\rho(\Gamma, t)$  approaches a local Gibbs distribution characterized by the hydrodynamic fields at its central point  $\mathbf{r}$ , such as is given by (5.4). However, this is not a solution to the Liouville equation due to the differences in hydrodynamic fields in different cells. The solution has additional fluxes driven by these gradients for subsequent

exchange of mass, energy, and momentum to equilibrate these fields to their uniform values (or to steady values if the system is driven). The first stage, approach to a universal form for the velocity distribution, occurs after a few collisions. This establishes the normal form of the solution where the hydrodynamic fields and their gradients characterize the state. Deviations from the Gibbs density are due to fluxes of mass, momentum, and energy across the cells. These fluxes are proportional to the differences in values of the fields (i.e., to their spatial gradients). The second stage is the evolution of the distribution through the changing values of the fields, according to the hydrodynamic equations.

This two-stage evolution can be expected for granular fluids as well. The initial velocity relaxation will not approach the local Gibbs density, but some other corresponding local normal state determined from the inelastic Liouville equation (see below). Subsequently, the deviations from this local normal state characterizing spatial inhomogeneities will again be via the macroscopic balance equations for the granular fluid. This is the space and time scale for a hydrodynamic description.

## VI. NAVIER-STOKES APPROXIMATION

The self-consistent solution to (5.8) and determination of  $N_\alpha(\mathbf{r}, t \mid \{y_\alpha\})$  is a formidable problem in general. Specific cases of interest may provide simplifications that allow further progress. Consider the example of uniform shear flow, where the system is driven by Lees - Edwards boundary conditions (simple periodic boundary conditions in the local Lagrangian frame [24]). At the macroscopic level this state is characterized by a uniform density and temperature, and a constant  $y$  derivative of  $U_x$  - the shear rate. This is an example for which all spatial gradients vanish, except the first order derivative of  $U_x$ . The latter can be small, so that all properties depend nonlinearly on the shear rate, but clearly the problem is considerably simplified.

The class of states to be considered here are those for which all spatial gradients of first order can occur, but which are small and all higher order derivatives are negligible. These are weakly inhomogeneous states. It is expected under these conditions that the normal solution to the Liouville equation can be represented by an expansion to first order in the gradients

$$\rho_n(\Gamma \mid \{y_\alpha\}) = \rho_{nl}(\Gamma \mid \{y_\alpha\}) + \mathbf{G}_\alpha(\Gamma, \mathbf{r} \mid \{y_\alpha\}) \cdot \nabla y_\alpha(\mathbf{r}, t) + \dots \quad (6.1)$$

The dots denote contributions from  $\nabla y_\alpha \nabla y_\alpha$ ,  $\nabla \nabla y_\alpha$  and higher order gradients. The reference state  $\rho_{h\ell}(\Gamma | \{y_\alpha\})$  is the *local homogeneous cooling state*, analogous to the local equilibrium state for a molecular fluid. As a normal state, it is a functional of the exact hydrodynamic fields  $\{y_\alpha\}$  and must yield the exact averages for the associated microscopic phase functions

$$\int d\Gamma (\rho_n - \rho_{h\ell}) a_\alpha = 0, \quad a_\alpha = (\hat{n}(\mathbf{r}), \hat{e}(\mathbf{r}), \hat{\mathbf{g}}(\mathbf{r})). \quad (6.2)$$

For spatially constant fields it must reduce to the HCS of (3.21)

$$\rho_h(\Gamma; \{y_{0\beta}\}) = \rho_{h\ell}(\Gamma | \{y_{0\beta} + \delta y_\beta\})|_{\delta y=0}, \quad \frac{\partial \rho_h}{\partial y_{0\alpha}} = \int d\mathbf{r} \frac{\delta \rho_{h\ell}(\Gamma | \{y_{0\beta} + \delta y_\beta\})}{\delta y_\alpha(\mathbf{r})} |_{\delta y=0}, \dots \quad (6.3)$$

where  $y_{0\alpha}$  denotes arbitrary homogeneous values. Thus, the choice for the local reference state is not arbitrary and other perturbations of the HCS consistent with (6.2) are not consistent with the second term of (6.1) being of first order in the gradients. Further characterization of the local HCS distribution is given in Appendix C. The determination of  $\mathbf{G}_\alpha(\Gamma, \mathbf{r} | \{y_\alpha\})$  is fixed by the requirement that (6.1) be a solution to the Liouville equation (5.8) to the same order in the gradients. This is discussed in the next section.

Small gradients means that the relative change in the hydrodynamic fields over the largest microscopic length scale  $\ell_0$  is small:  $\ell_0 \partial_r \ln y_\alpha \ll 1$ . There are two characteristic length scales, the mean free path and the grain diameter. For a dilute gas the mean free path is largest, while for a dense fluid the grain size is largest. In many cases, the condition for small gradients can be determined by control over the initial or boundary conditions and it turns out to be the usual experimental condition for simple normal fluids. As noted in the introduction, some special states for granular fluids entail a balance of the intrinsic internal cooling and the boundary or initial conditions such that control over the gradients is lost (two examples are noted in the discussion). Thus a careful analysis of each case is required before making the assumption of small gradients. In the following it is assumed this has been assured.

The constitutive equations follow from substitution of (6.1) into (5.5)-(5.7)

$$\zeta(\mathbf{r}, t | \{y_\alpha\}) \rightarrow \zeta_\ell(\mathbf{r}, t | \{y_\alpha\}) + \frac{2}{3n(\mathbf{r}, t)T(\mathbf{r}, t)} \int d\Gamma w(\mathbf{r}) \mathbf{G}_\alpha(\Gamma | \{y_\alpha\}) \cdot \nabla y_\alpha(\mathbf{r}, t) \quad (6.4)$$

$$\mathbf{q}(\mathbf{r}, t | \{y_\alpha\}) \rightarrow \mathbf{q}_\ell(\mathbf{r}, t | \{y_\alpha\}) + \int d\Gamma \mathbf{s}'(\mathbf{r}) \mathbf{G}_\alpha(\Gamma | \{y_\alpha\}) \cdot \nabla y_\alpha(\mathbf{r}, t) \quad (6.5)$$

$$P_{\alpha\beta}(\mathbf{r}, t \mid \{y_\alpha\}) \rightarrow P_{\ell\alpha\beta}(\mathbf{r}, t \mid \{y_\alpha\}) + \int d\Gamma h'_{\alpha\beta}(\mathbf{r}) \mathbf{G}_\nu(\Gamma \mid \{y_\alpha\}) \cdot \nabla y_\nu(\mathbf{r}, t) \quad (6.6)$$

The subscript  $\ell$  on the first terms denote their local HCS averages, i.e. (5.5)-(5.7) evaluated with  $\rho_n(\Gamma \mid \{y_\alpha\}) \rightarrow \rho_{h\ell}(\Gamma \mid \{y_\alpha\})$ . By construction, these constitutive relations are correct to first order in the gradients. However, the fields at different space points of the functional also differ by terms of first order in the gradients. Therefore, when an average at some chosen space point is calculated a further simplification is possible by retaining only terms of linear order in gradients at that point. To illustrate, consider some local property represented by  $a(\Gamma, \mathbf{r})$ . Its local HCS average can be evaluated to first order using

$$\begin{aligned} \rho_{h\ell} &= \rho_h(\{y_\alpha(\mathbf{r}, t)\}) + \int d\mathbf{r}' \left( \frac{\delta \rho_{h\ell}}{\delta y_\beta(\mathbf{r}', t)} \right)_{\delta y=0} (y_\beta(\mathbf{r}', t) - y_\beta(\mathbf{r}, t)) + \dots \\ &= \rho_h(\{y_\alpha(\mathbf{r}, t)\}) + \left( \mathbf{M}_\nu(\{y_\alpha(\mathbf{r}, t)\}) - \mathbf{r} \frac{\partial \rho_h(\{y_\alpha(\mathbf{r}, t)\})}{\partial y_\alpha(\mathbf{r}, t)} \right) \cdot \nabla y_\beta(\mathbf{r}, t) + \dots \end{aligned} \quad (6.7)$$

where the dots denote terms of higher order in the gradients, and  $\mathbf{M}_\nu$  is defined by

$$\mathbf{M}_\nu = \int d\mathbf{r}' \left( \frac{\delta(\rho_{\ell n})}{\delta y_\nu(\mathbf{r}', t)} \right)_{\delta y=0} \mathbf{r}' \quad (6.8)$$

Then the average of  $a(\Gamma, \mathbf{r})$  becomes

$$\begin{aligned} \int d\Gamma a(\Gamma, \mathbf{r}) \rho_{h\ell}(\Gamma \mid \{y_\alpha(\mathbf{r}, t) + \delta y_\alpha\}) &\rightarrow \frac{1}{V} \int d\Gamma A(\Gamma) \rho_h(\Gamma, \{y_\alpha(\mathbf{r}, t)\}) \\ &\quad + \int d\Gamma a(\Gamma, \mathbf{0}) \mathbf{M}_\beta \cdot \nabla y_\beta(\mathbf{r}, t) \end{aligned} \quad (6.9)$$

The first term is the local HCS functional evaluated at the "constant" value of  $\{y_\alpha(\mathbf{r}, t)\}$ , in which case it becomes the HCS cooling function of these values, according to (6.3),  $\rho_{h\ell}(\Gamma \mid \{y_\alpha(\mathbf{r}, t)\}) = \rho_h(\Gamma, \{y_\alpha(\mathbf{r}, t)\})$ . The second term is the contribution from  $\delta y_\alpha(\mathbf{r}', t)$  which is of first order in the gradient  $\nabla y_\nu(\mathbf{r}, t)$ .

The first terms on the right sides of (6.4)-(6.6) therefore have two terms at this order, one evaluated at the HCS and the second of first order in the gradient. These latter combine with the second terms of (6.4)-(6.6). These expressions then have their final forms to first order in the gradients

$$\zeta(\mathbf{r}, t \mid \{y_\alpha\}) \rightarrow \zeta_h(\{y_\alpha(\mathbf{r}, t)\}) + \zeta_U(\{y_\alpha(\mathbf{r}, t)\}) \nabla \cdot \mathbf{U}(\mathbf{r}, t) \quad (6.10)$$

$$\mathbf{q}(\mathbf{r}, t \mid \{y_\alpha\}) \rightarrow -\lambda(\{y_\alpha(\mathbf{r}, t)\}) \nabla T(\mathbf{r}, t) - \mu(\{y_\alpha(\mathbf{r}, t)\}) \nabla n(\mathbf{r}, t) \quad (6.11)$$

$$P_{\alpha\beta}(\mathbf{r}, t \mid \{y_\alpha\}) \rightarrow p_h(\{y_\alpha(\mathbf{r}, t)\})\delta_{\alpha\beta} - \kappa(\{y_\alpha(\mathbf{r}, t)\})\nabla \cdot \mathbf{U}(\mathbf{r}, t)\delta_{\alpha\beta} - \eta(\{y_\alpha(\mathbf{r}, t)\})\left(\partial_\alpha U_\beta(\mathbf{r}, t) + \partial_\beta U_\alpha(\mathbf{r}, t) - \frac{2}{3}\nabla \cdot \mathbf{U}(\mathbf{r}, t)\delta_{\alpha\beta}\right) \quad (6.12)$$

Fluid symmetry (rotational invariance of  $\rho_h$ ) has been used to recognize  $\mathbf{q}_h(\mathbf{r}, t \mid \{y_\alpha\}) = 0$ , and that contributions to the scalar  $\zeta$  from gradients of the density and temperature must vanish. Similarly, contributions to the vector  $\mathbf{q}$  from velocity gradients must vanish, and no second order tensor contributions to  $P_{\alpha\beta}$  can be constructed from density and temperature gradients. Equation (6.12) has the familiar form of Newton's viscosity law, while (6.11) is Fourier's law with an additional contribution from the density gradient.

These results, together with the macroscopic balance equations (4.12)-(4.14) provide the closed set of hydrodynamic equations with constitutive relations calculated determined to first order in the gradients. "Determined" means that formally exact expressions are now available for calculation all parameters in these equations. For example,  $p_h$  and  $\zeta_h$  are properties of the HCS

$$p_h(\{y_\alpha\}) = \frac{1}{3V} \int d\Gamma \rho_h(\Gamma; \{y_\alpha\}) H'_{\alpha\alpha}, \quad H'_{\alpha\alpha} = \int d\mathbf{r} h'_{\alpha\alpha}(\mathbf{r}). \quad (6.13)$$

$$\zeta_h(\{y_\alpha\}) = \frac{2}{3nTV} \int d\Gamma \rho_h(\Gamma; \{y_\alpha\}) W_\zeta, \quad W_\zeta = \int d\mathbf{r} w'(\mathbf{r}) \quad (6.14)$$

Recall that a prime on the phase function denotes the local rest frame,  $\mathbf{v}_s \rightarrow \mathbf{V}_s = \mathbf{v}_s - \mathbf{U}_s(\mathbf{r}, t)$ . Equation (6.13) now defines the hydrostatic pressure for a granular fluid as a function of the local density and temperature. The scaling property of  $\rho_h$  displayed in (3.21) confirm that  $p_h(\{y_\alpha\}) \propto T$  and  $\zeta_h \propto T^{1/2}$ . Similarly, expressions for the transport coefficients  $\zeta_U$ ,  $\lambda$ ,  $\mu$ ,  $\kappa$ , and  $\eta$  as phase space averages follow from this analysis. Their explicit expressions are deferred to the next section.

It is appropriate to register at this point the explicit form for the full nonlinear granular Navier - Stokes equations [25]

$$D_t n + n \nabla_{\mathbf{r}} \cdot \mathbf{U} = 0 \quad (6.15)$$

$$(D_t + \zeta_h) T + \frac{2}{3n} \left( p + \frac{3nT}{2} \zeta_U + \left( \frac{2}{3} \eta - \kappa \right) \nabla \cdot \mathbf{U} \right) \nabla \cdot \mathbf{U} - \frac{2}{3n} (\eta (\partial_\alpha U_\beta + \partial_\beta U_\alpha) \partial_\alpha U_\beta + \nabla \cdot (\lambda \nabla T + \mu \nabla n)) = 0, \quad (6.16)$$

$$D_t U_\alpha + (mn)^{-1} \partial_\alpha \left( p - \left( \frac{2}{3} \eta + \kappa \right) \nabla \cdot \mathbf{U} \right) - (mn)^{-1} \partial_\beta \eta (\partial_\alpha U_\beta + \partial_\beta U_\alpha) = 0, \quad (6.17)$$



These are almost the same as the Navier-Stokes equations for a molecular fluid, except for the presence of the cooling rate  $\zeta_h$  and two new transport coefficients,  $\zeta_U$  and  $\mu$  in the temperature equation. Perhaps the most significant of these is the cooling rate, which leads to new instabilities and new stationary states. To illustrate, consider small homogeneous perturbations  $\{\delta y_\alpha\}$  of the HCS solution. The linear equations for the perturbations are

$$\partial_t n = 0 = \partial_t \delta U_\alpha, \quad \left( \partial_t + \zeta_{0h} + T_h \frac{\partial \zeta_{0h}}{\partial T_h} \right) \delta T + T_h \frac{\partial \zeta_{0h}}{\partial n_h} \delta n = 0 \quad (6.18)$$

Using the scaling  $\zeta_{0h} \propto \sqrt{T_h}$ , and introducing the dimensionless variables  $\delta T^* / \delta T / T_h$ ,  $\delta U_\alpha^* = \delta U_\alpha / v_h(t)$ , these become linear equations with time independent coefficients that are easily solved. It is found that there is one decaying mode, one constant mode, and three growing modes. A similar result is found for finite spatial gradients, where the same modes are unstable at sufficiently long wavelengths. A second interesting effect of the cooling rate is the existence of new steady states, that are possible when external work done on the system or energy input is balanced by the inherent cooling from collisions. For example, the temperature equation for steady, simple shear flow becomes

$$\zeta_h = \frac{2}{3nT} \eta \partial_y U_x. \quad (6.19)$$

It is noted in the discussion that for many of these steady states, it is not possible to control the size of the spatial gradients and higher order hydrodynamic effects beyond Navier-Stokes order are required.

To summarize, a hydrodynamic description for normal and granular fluids has been given from the exact macroscopic balance equations and the assumption of a normal solution to the Liouville equation. For the class of fluid states with small spatial gradients in the hydrodynamic fields, this normal solutions is constructed to leading order in the form (6.1) which provides constitutive relations in terms of the fields and their gradients. In this way, the macroscopic balance equations become a closed set of hydrodynamic equations. The parameters of this description (e.g., pressure, transport coefficients) are given in terms of averages over the solution (6.1). It remains to make that solution more explicit and this is the topic of the next section.

## VII. CONSTRUCTION OF THE NORMAL SOLUTION AND TRANSPORT COEFFICIENTS

The objective now is to construct a solution of the form (6.1) that is exact up through first order in the gradients. This extends recent results for a corresponding solution to the Liouville equation resulting from small initial perturbations of the HCS [11, 12]. In that case the linearized Navier-Stokes equations are obtained for states close to strictly homogeneous systems. Here that assumption holds only locally, so the full nonlinear Navier-Stokes equations result. The transport coefficients obtained by both methods are the same, except for the values of the fields on which they depend.

As described above, the ultimate use of this solution is to calculate local properties of the form

$$A(\mathbf{r} \mid \{y_\alpha(t)\}) = \int d\Gamma a(\Gamma, \mathbf{r}) \rho_n(\Gamma \mid \{y_\alpha(\mathbf{r}, t) + \delta y_\alpha(t)\}). \quad (7.1)$$

Therefore, in the following analysis the gradient expansion are referred to the field point  $\mathbf{r}$  of interest,  $y_\alpha = y_\alpha(\mathbf{r}) + \delta y_\alpha$ . Of course the results will be general and applicable to any choice for  $\mathbf{r}$ . Consider first a general solution of the form

$$\rho(\Gamma, t \mid \{y_\alpha(t)\}) = \rho_{h\ell}(\Gamma \mid \{y_\alpha(t)\}) + \Delta(\Gamma, t \mid \{y_\alpha(t)\}). \quad (7.2)$$

The notation makes explicit the fact that there is both explicit time dependence and that which occurs through  $\{y_\alpha(\mathbf{r}, t)\}$  in both  $\rho$  and  $\Delta$ , while  $\rho_{h\ell}$  depends on  $t$  only through  $\{y_\alpha(\mathbf{r}, t)\}$  by construction. The Liouville equation gives

$$\partial_t \Delta + \int d\mathbf{r} \frac{\delta \Delta}{\delta y_\alpha(\mathbf{r}, t)} N_\alpha(\mathbf{r}, t \mid \{y_\alpha(t)\}) + \bar{L} \Delta = - \int d\mathbf{r} \frac{\delta \rho_{h\ell}}{\delta y_\alpha(\mathbf{r}, t)} N_\alpha(\mathbf{r}, t \mid \{y_\alpha(t)\}) - \bar{L} \rho_{h\ell}. \quad (7.3)$$

It is understood here that the time derivative is taken at constant  $\{y_\alpha(\mathbf{r}, t)\}$ . It is expected that on some time scale this time dependence goes to zero and (7.3) becomes the same as (5.8) for a normal solution.

An approximate solution is sought by expanding in the gradients. The right side of (7.3) is evaluated in Appendix E with the result

$$\partial_t \Delta + \int d\mathbf{r} \frac{\delta \Delta}{\delta y_\alpha(\mathbf{r}, t)} N_\alpha(\mathbf{r}, t \mid \{y_\alpha(t)\}) + (1 - \mathcal{P}) \bar{L} \Delta = - (1 - \mathcal{P}) \Upsilon_\nu(\Gamma, \{y_\alpha(\mathbf{r}, t)\}) \cdot \nabla y_\nu(\mathbf{r}, t) \quad (7.4)$$

with "fluxes"  $\Upsilon_\nu$  given by

$$\begin{aligned}\Upsilon_\nu(\Gamma, \{y_\alpha(\mathbf{r}, t)\}) &\equiv (\bar{\mathcal{L}}_T \delta_{\nu\mu} - K_{\nu\mu}^T(\{y_\alpha(\mathbf{r}, t)\}) \mathbf{M}_\mu(\Gamma, \{y_\alpha(\mathbf{r}, t)\})) \\ \mathbf{M}_\nu(\Gamma, \{y_\alpha(\mathbf{r}, t)\}) &= \int d\mathbf{r} \left( \frac{\delta \rho_{h\ell}(\Gamma | \{y_\alpha(t)\})}{\delta y_\alpha(\mathbf{r}, t)} \right)_{\delta y=0} \mathbf{r}.\end{aligned}\quad (7.5)$$

Also  $\bar{\mathcal{L}}_T$  is the operator of (3.27) with  $T_h$  replaced by  $T(\mathbf{r}, t)$  and  $K^T$  is the transpose of the matrix

$$K = \begin{pmatrix} 0 & 0 & 0 \\ \frac{\partial(\zeta_h T)}{\partial n} & \frac{\partial(\zeta_h T)}{\partial T} & 0 \\ 0 & 0 & 0 \end{pmatrix}.\quad (7.6)$$

The matrix  $K$  generates the solution for homogeneous perturbations of the hydrodynamic equations

$$\begin{aligned}\partial_t \delta y_\nu(t) &= N_\nu(\mathbf{r}, t | \{y_\alpha(\mathbf{r}, t) + \delta y_\alpha(t)\}) - N_\nu(\mathbf{r}, t | y_\alpha(\mathbf{r}, t)) \\ &\rightarrow -K_{\nu\mu}(\{y_\alpha(\mathbf{r}, t)\}) \delta y_\mu(t).\end{aligned}\quad (7.7)$$

Further interpretation of its occurrence here is given below. There are two important observations that are a consequence of the special choice of  $\rho_{h\ell}$  as the reference state. First, the right side of (7.4) is proportional to the gradients. This admits solutions of the form (6.1)

$$\Delta(\Gamma, t | \{y_\alpha(t)\}) \rightarrow \mathbf{G}_\alpha(\Gamma, t, \{y_\alpha(\mathbf{r}, t)\}) \cdot \nabla y_\alpha(\mathbf{r}, t).\quad (7.8)$$

The second observation is the occurrence of the orthogonal projection  $(1 - \mathcal{P})$ , defined below, which excludes the invariants of the generator for dynamics in (7.4). This will be shown to be essential for the existence of a normal solution.

Substitution of the form (7.8) into (7.4) leads to an equation for  $\mathbf{G}_\alpha$  (see Appendix E for details)

$$\partial_t \mathbf{G}(t) + (1 - \mathcal{P})(I\bar{\mathcal{L}}_T + K^T) \mathbf{G}(t) = -(1 - \mathcal{P}) \Upsilon,\quad (7.9)$$

where a compact matrix notation has been introduced. The time derivative is again taken at constant  $\{y_\alpha(\mathbf{r}, t)\}$  and the dependence on these fields has been suppressed since they are simply parameters of the equation. Integrating this equation with the choice  $\mathbf{G}(0) = 0$  (initial local HCS) gives the formal solution

$$\mathbf{G}(t) = -(1 - \mathcal{P}) \int_0^t dt' e^{-(I\bar{\mathcal{L}}_T + K^T)t'} (1 - \mathcal{P}) \Upsilon.\quad (7.10)$$

Use has been made of the property

$$(1 - \mathcal{P}) (I\bar{\mathcal{L}}_T + K^T) \mathcal{P} = 0, \quad (7.11)$$

which is also proved in the Appendix.

To interpret the role of  $(1 - \mathcal{P})$  in these expressions, defined in (7.16) below, consider the average of some property represented by  $X(\Gamma)$

$$\langle X; t \rangle = \langle X \rangle_{hl} + \left( \int_0^t dt' \mathbf{C}_\nu^X(t') \right) \cdot \nabla y_\nu \quad (7.12)$$

where the first term is the local HCS average and the correlation function  $\mathbf{C}_\nu(t)$  is

$$\mathbf{C}_\nu^X(t) = - \int d\Gamma X(\Gamma) (1 - \mathcal{P}) \left( e^{-(I\bar{\mathcal{L}}_T + K^T)t} (1 - \mathcal{P}) \Upsilon(\Gamma) \right)_\nu. \quad (7.13)$$

The only explicit time dependence on the right side of (7.12) occurs in the upper limit of the time integral. Suppose that  $\mathbf{C}_\nu^X(t) \rightarrow 0$  for  $t \gg t_m$ . Then for  $t \gg t_m$  the upper limit of the time integral can be extended to  $\infty$  and the average of  $X$  becomes normal - all of its time dependence is through the parameters  $\{y_\alpha(\mathbf{r}, t)\}$

$$\langle X; t \rangle \rightarrow \langle X \rangle_n = \langle X \rangle_{hl} + \left( \int_0^\infty dt' \mathbf{C}_\nu^X(t') \right) \cdot \nabla y_\nu \quad (7.14)$$

Thus  $t_m$  sets the time scale for the normal solution, and hence for the onset of hydrodynamics. A necessary condition for the existence of a  $t_m$  is the convergence of the time integral in (7.14). This means there should be no invariants of the generator for time dependence,  $I\bar{\mathcal{L}}_T + K^T$  in its domain of action. It is shown in Appendix E that such invariants exist

$$(I\bar{\mathcal{L}}_T + K^T) \Psi = 0, \quad \Psi_\nu = \frac{\partial \rho_h(\{y_\alpha\})}{\partial y_\nu}. \quad (7.15)$$

The existence of these invariants of (7.15) provide a microscopic representation of these long wavelength hydrodynamic excitations at long wavelength in the spectrum of  $\bar{\mathcal{L}}_T$  [19]. The effective generator for the dynamics,  $\bar{\mathcal{L}}_T + K^T$ , gives a dynamics with these homogeneous perturbations subtracted out. However, the projection operator  $(1 - \mathcal{P})$  projects out such contributions from the definition (E24)

$$(1 - \mathcal{P}) X = X - \Psi_\alpha \frac{1}{V} \int d\Gamma \tilde{A}_\alpha X, \quad \frac{1}{V} \int d\Gamma \tilde{A}_\alpha \Psi_\beta = \delta_{\alpha\beta}. \quad (7.16)$$

The biorthogonal set  $\tilde{A}_\alpha$  are linear combinations of the total particle number, energy, and momentum defined in (E19). According to (7.7)  $K$  is the generator for homogeneous hydrodynamic perturbations.

A technical complication is the occurrence of period time dependence, the Poincare recurrence time. This can be removed by considering the thermodynamic limit of  $V \rightarrow \infty$ ,  $N \rightarrow \infty$  at constant  $N/V$ . Therefore, the normal solution to the Liouville equation to first order in the gradients is written

$$\rho_n(\Gamma | \{y_\alpha(t)\}) = \rho_{he}(\Gamma | \{y_\alpha(t)\}) - \left( \lim \int_0^t dt' e^{-(I\bar{\mathcal{L}}_T + K^T)t'} (1 - \mathcal{P}) \Upsilon \right)_\nu \cdot \nabla y_\nu. \quad (7.17)$$

It is understood that the limit is taken in the context of an average like (7.14) with the thermodynamic limit followed by the long time limit, all at constant  $\{y_\alpha\} = \{y_\alpha(\mathbf{r}, t)\}$ .

The constitutive equations now follow directly from (6.4) - (6.6) and fluid symmetry to get the final forms (6.10) - (6.12) with the transport coefficients identified as

$$\zeta_U(\{y_\alpha\}) = \frac{2}{3nTV} \int d\Gamma W^- \mathbf{M}_{3xx} + \lim \int_0^t dt' C_\nu^\zeta(t') \quad (7.18)$$

$$\lambda(\{y_\alpha\}) = \frac{1}{3V} \int d\Gamma \mathbf{S}^- \cdot \mathbf{M}_2 + \lim \int_0^t dt' C_\nu^\lambda(t') \quad (7.19)$$

$$\mu(\{y_\alpha\}) = \frac{1}{3V} \int d\Gamma \mathbf{S}^- \cdot \mathbf{M}_1 + \lim \int_0^t dt' C^\mu(t') \quad (7.20)$$

$$\eta(\{y_\alpha\}) = \frac{1}{V} \int d\Gamma H_{xy}^- M_{3xy} + \lim \int_0^t dt' C^\eta(t') \quad (7.21)$$

$$\kappa(\{y_\alpha\}) = \frac{1}{3V} \int d\Gamma H_{xx}^- M_{3xx} + \lim \int_0^t dt' C^\kappa(t') \quad (7.22)$$

with the correlation functions

$$C^\zeta(t') = -\frac{2}{3nTV} \int d\Gamma \widetilde{W} e^{-(\bar{\mathcal{L}} - \lambda_3)t'} \left( e^{-(I\bar{\mathcal{L}}_T + K^T)t'} (1 - \mathcal{P}) \Upsilon \right)_{3xx} \quad (7.23)$$

$$C^\lambda(t') = -\frac{1}{3V} \int d\Gamma \widetilde{\mathbf{S}} \cdot \left( e^{-(I\bar{\mathcal{L}}_T + K^T)t'} (1 - \mathcal{P}) \Upsilon \right)_2 \quad (7.24)$$

$$C^\mu(t') = -\frac{1}{3V} \int d\Gamma \widetilde{\mathbf{S}} \cdot \left( e^{-(I\bar{\mathcal{L}}_T + K^T)t'} (1 - \mathcal{P}) \Upsilon \right)_1$$

$$C^\eta(t') = -\frac{1}{V} \int d\Gamma \widetilde{H}_{xy} \left( e^{-(I\bar{\mathcal{L}}_T + K^T)t'} (1 - \mathcal{P}) \Upsilon \right)_{3xy} \quad (7.25)$$

$$C^\kappa(t') = -\frac{1}{3V} \int d\Gamma H_{xx}^- \left( e^{-(I\bar{\mathcal{L}}_T + K^T)t'} (1 - \mathcal{P}) \Upsilon \right)_{3xx} \quad (7.26)$$

and

$$\widetilde{W} = \int d\mathbf{r} (1 - \mathcal{P}^\dagger) w(\mathbf{r}), \quad \widetilde{\mathbf{S}} = \int d\mathbf{r} (1 - \mathcal{P}^\dagger) \mathbf{s}'(\mathbf{r}), \quad \widetilde{H}_{ij} = \int d\mathbf{r} (1 - \mathcal{P}^\dagger) h'_{ij}(\mathbf{r}) \quad (7.27)$$

The adjoint projection operator  $\mathcal{P}^\dagger$  is defined by  $\int d\Gamma X \mathcal{P} Y \equiv \int d\Gamma (\mathcal{P}^\dagger X) Y$ . The first terms of (7.18) - (7.22) come from the expansion of  $\rho_{h\ell}$  to first order in the gradients, (6.7). They vanish for non-singular, conservative forces but are non-zero for granular fluids and for the elastic hard sphere fluid. Also, they vanish in the low density limit but can be dominant at high densities.

The appearance of  $\bar{\mathcal{L}}_T$  in (7.9), (7.17) and the correlation functions for the transport coefficients is awkward as it implies using the temperature as a dynamical variable in addition to the phase space variables  $\Gamma$ . This difficulty can be avoided by transforming to the dimensionless representation described at the end of Section III. The transformation is described in Appendix E with the results

$$\left( \partial_s + (1 - \mathcal{P}^*) \left( I\bar{\mathcal{L}}^* - \Lambda^* \right) \right) \mathbf{G}^* = - (1 - \mathcal{P}^*) \left( I\bar{\mathcal{L}}^* - \Lambda^* \right) \mathbf{M}^* (\{y_\alpha\}), \quad (7.28)$$

where an asterisk denotes the function, operator, or matrix expresses in terms of the dimensionless variables. The matrix  $\Lambda^*$  is

$$\Lambda^* = \begin{pmatrix} 0 & \frac{\partial(\zeta_h T)}{T v_h \ell^2 \partial n} & 0 \\ 0 & \frac{1}{2} \zeta_h^* & 0 \\ 0 & 0 & -\frac{1}{2} \zeta_h^* \end{pmatrix}. \quad (7.29)$$

Note that now  $\bar{\mathcal{L}}_T$  has been replaced by the phase space operator  $\bar{\mathcal{L}}$  of (3.27) and the temperature no longer appears in this dimensionless form. The variable  $s$  is the same as that of (3.35), with  $T_h \rightarrow T$ , and represents the average number of collisions per particle. The corresponding solution to the dimensionless Liouville equation is

$$\rho_n^*(s, \Gamma^* | \{y_\alpha^*(t)\}) = \rho_{h\ell}^*(\Gamma^* | \{y_\alpha^*(s)\}) - \left( \lim \int_0^s ds' \left( e^{-(I\bar{\mathcal{L}}^* - \Lambda^*)s'} (1 - \mathcal{P}^*) \mathbf{r}^* \right)_\nu \right) \cdot \nabla^* y_\nu^*. \quad (7.30)$$

The eigenvalues of  $\Lambda$  are  $0, \frac{1}{2}\zeta_h^*, -\frac{1}{2}\zeta_h^*$ . These are excitations for small homogeneous perturbations of the hydrodynamic equations in this representation. The invariants of (7.15) become

$$\left( I\bar{\mathcal{L}}^* - \Lambda^* \right) \Psi^* = 0. \quad (7.31)$$

The interpretation of  $(1 - \mathcal{P}^*)$  excluding these invariants of the dynamics is the same as discussed above. For practical purposes, both in theoretical and simulation applications, it is usually most convenient to use the dimensionless forms.

This completes the formal derivation of the nonlinear Navier-Stokes equations, including expressions for the pressure tensor, cooling rate, and energy flux including contributions up through first order in the gradients of the hydrodynamic fields. These expressions are functions of the hydrodynamic fields to be determined by their detailed calculation. The scaling property of hard spheres allows the temperature dependence to be obtained directly from dimensional analysis, but the density dependence requires confrontation of the full many-body problem for calculation.

### A. Example: Shear Viscosity

To illustrate the results for the transport coefficients, the shear viscosity is considered in more detail. The dimensionless form is used, but to simplify the notation the asterisk is suppressed. The shear viscosity is found to be

$$\eta(\{y_\alpha\}) = \frac{1}{V} \int d\Gamma H_{xy} M_\eta - \lim \frac{1}{V} \int_0^s ds' \int d\Gamma H_{xy} e^{-(\bar{\mathcal{L}} - \lambda_3)s'} \Upsilon_\eta. \quad (7.32)$$

with  $\lambda_3 = -\frac{1}{2}\zeta_h$  and

$$M_\eta = -\frac{1}{2} \sum_{s=1}^N q_{xs} \partial_{v_{ys}} \rho_h, \quad \Upsilon_\eta = (\bar{\mathcal{L}} - \lambda_3) M_\eta. \quad (7.33)$$

The projection operators vanish in this case from fluid symmetry. The volume integrated momentum flux  $H_{xy}$  is given from (B14) as

$$H_{xy} = \sum_{r=1}^N v_{rx} v_{ry} - \frac{1}{2} \sum_{r,s} q_{rsx} T(r, s) v_{sy}. \quad (7.34)$$

In the elastic limit

$$(\bar{\mathcal{L}} - \lambda_3) \rightarrow \bar{L}, \quad \rho_h \rightarrow \rho_e, \quad \Upsilon_\eta \rightarrow -H_{xy}^- \rho_e, \quad M_\eta \rightarrow -\frac{1}{2} \sum_{s=1}^N q_{xs} v_{ys}, \quad (7.35)$$

This result for the flux  $\Upsilon_\eta$  follows from (A21)

$$\Upsilon_\eta \rightarrow \bar{L} (M_\eta \rho_e) = (M_\eta \bar{L} \rho_e) + (L_- M_\eta) \rho_e = -H_{xy}^- \rho_e. \quad (7.36)$$

Interestingly, this introduces the generator for time reversed dynamics and the associated momentum flux  $H_{xy}^-$ . The expression for the shear viscosity becomes

$$\eta(\{y_\alpha\}) \rightarrow \frac{1}{V} \int d\Gamma H_{xy} M_{3xy} + \lim \frac{1}{V} \int_0^s ds' \int d\Gamma H_{xy} e^{-\bar{L}s'} H_{xy}^-. \quad (7.37)$$

This is the Green-Kubo shear viscosity for a normal fluid. It differs from that for a fluid whose particles interact via non-singular forces by the presence of the first term on the right side, and by the difference between the two fluxes (forward and reversed dynamics) in the flux-flux time correlation function. As noted above, this is a peculiarity of non-conservative and/or singular forces.

Comparison of (7.32) and (7.37) shows the most significant new affects of dissipative dynamics: 1) one of the fluxes,  $\Upsilon_\eta$  is generated from the reference homogeneous state. This representation holds as well for normal fluids, but for granular fluids the homogeneous state is no longer given by an equilibrium distribution. Hence the form of the flux is quite different from that for a normal fluid; 2) the generator of the dynamics,  $(\overline{\mathcal{L}} - \lambda_3)$ , is modified in two important ways. The operator  $\overline{\mathcal{L}}$  generates the usual hard sphere trajectories, but modified by an additional scaling operator to account for the dominant effects of collisional cooling. In addition, the dynamics of homogeneous perturbations of the reference state are compensated by the subtraction of an appropriate eigenvalue for that dynamics,  $\lambda_3$ . This effectively shifts the spectrum of  $(\overline{\mathcal{L}} - \lambda_3)$  to exclude the homogeneous dynamics of the reference state - cooling and its homogeneous perturbations.

## B. Impurity Diffusion

Perhaps the simplest example of hydrodynamics is the diffusion of an impurity particle in a host fluid. To illustrate briefly, the host fluid is taken to be in its HCS and unperturbed by a single impurity particle. The impurity is taken to be a hard sphere, although its mass, size and restitution coefficient for collisions with particles of the host fluid may be different from those for fluid particle pairs. The macroscopic balance equation is that for conservation of the probability density  $P(\mathbf{r}, t)$  for the location of the impurity at time  $t$

$$\partial_t P(\mathbf{r}, t) + \nabla \cdot \mathbf{J}(\mathbf{r}, t) = 0. \quad (7.38)$$

This follows from averaging the corresponding microscopic conservation law, where  $P(\mathbf{r}, t)$  and the flux  $\mathbf{J}(\mathbf{r}, t)$  are

$$P(\mathbf{r}, t) = \langle \delta(\mathbf{r} - \mathbf{q}_0); t \rangle, \quad \mathbf{J}(\mathbf{r}, t) = \langle \mathbf{v}_0 \delta(\mathbf{r} - \mathbf{q}_0); t \rangle. \quad (7.39)$$



The subscript zero distinguishes the position and velocity of the impurity particle. The average flux  $\mathbf{J}(\mathbf{r}, t)$  is given by Fick's law in the hydrodynamic limit and for small gradients

$$\mathbf{J}(\mathbf{r}, t) \rightarrow -D(\{y_\alpha\})\nabla P(\mathbf{r}, t). \quad (7.40)$$

The above analysis can be applied directly to this case as well with the resulting Green-Kubo expression for the dimensionless diffusion coefficient [13] (asterisks suppressed)

$$D = \lim \frac{mT_0}{2m_0T} \int_0^s ds' C_{vv}(s'). \quad (7.41)$$

The normalized velocity autocorrelation function is

$$C_{vv}(s) \equiv \frac{\langle \mathbf{v}_0(s) \cdot \mathbf{v}_0 \rangle}{\langle v_0^2 \rangle} = \frac{2m_0T}{3mT_0} \int d\Gamma (e^{s\mathcal{L}}\mathbf{v}_0) \cdot \mathbf{v}_0 \rho_{hcs}. \quad (7.42)$$

This expression for the diffusion coefficient is very similar to the corresponding result for normal fluids except for the changes noted above for the shear viscosity - a different generator for the dynamics and a different reference fluid state. In addition, the appearance of two different temperatures here is due to the different mechanical properties of the host and impurity particles (e.g., mass, size, restitution coefficient). This is a reflection of the failure of equipartition for granular mixtures, as is expected for any non equilibrium state [26].

A simple estimate for the diffusion coefficient can be obtained from truncation of the cumulant expansion for the correlation function [13, 27]

$$C_{vv}(s) = \exp \left[ \sum_{p=1}^{\infty} \frac{1}{p!} \omega_p (-s)^p \right] \rightarrow e^{-\omega_1 s} \quad (7.43)$$

where the first cumulant is

$$\omega_1 = -\frac{\langle (\mathcal{L}\mathbf{v}_0) \cdot \mathbf{v}_0 \rangle}{\langle v_0^2 \rangle} \rightarrow -\frac{1}{2}\zeta_h + \nu \left( 1 + \frac{mT_0}{m_0T} \right)^{1/2}. \quad (7.44)$$

The arrow indicates an evaluation of the average using the first term in an expansion of the reduced pair distribution function for the impurity and host particle in Sonine polynomials, and a neglect of velocity correlations. The dimensionless collision frequency  $\nu$  and cooling rate  $\zeta_h$  evaluated in the same approximation are

$$\nu = \frac{2\pi(1+\alpha_0)}{3\Gamma(3/2)} \frac{m}{m+m_0} \left( \frac{\bar{\sigma}}{\sigma} \right)^2 \chi_0, \quad \zeta_h = \frac{2^{1/2}\pi}{3\Gamma(3/2)} \chi(1-\alpha^2), \quad (7.45)$$

and  $\chi_0$  is the pair correlation function at contact. This gives the diffusion coefficient as

$$D \rightarrow \lim \frac{mT_0}{m_0T} \left( 2 \left( 1 + \frac{mT_0}{m_0T} \right)^{1/2} \nu - \zeta_h \right)^{-1} (1 - e^{-\omega_1 s}). \quad (7.46)$$

It is seen that  $t_m = \omega_1^{-1}$  sets the time scale for cross over to a normal solution and hydrodynamics.

This result has been compared with molecular dynamics simulations for the special case of self-diffusion (mechanically equivalent particles) [13]. It is found to give excellent agreement at low densities and weak inelasticity, while differences grow at both higher densities and stronger inelasticity. This result also agrees with the Enskog kinetic theory for both normal and granular gases.

## VIII. KINETIC THEORY AND BOLTZMANN LIMIT

The above analysis has provided an exact formal derivation of the hydrodynamic equations and associated expressions for the transport coefficients in terms of HCS correlation functions. The difficult many-body problem is postponed to the final stage of evaluating these expressions. Approximations are introduced only at this final stage. An alternative approach is that of kinetic theory where the many-body problem is confronted at the outset, and approximations introduced at an early stage. Of course, the two should yield equivalent results to the extent that consistent approximations are used in each. In this section, the ideas behind a kinetic theory derivation of the hydrodynamic equations are reviewed and an approximation expected to be valid for low density gases is introduced. Although attention is focused here on low density, kinetic theory methods with different approximations can be applied to higher density fluids as well; for references to granular gases see [28]. The macroscopic balance equations are obtained from the resulting kinetic equation, and the associated constitutive equations are expressed in terms of the solution to that equation. The construction of a normal solution is described in analogy to that given above for the Liouville equation, and expressions for the transport coefficients of a low density gas are obtained.

The motivation for a kinetic theory representation is based on the fact that hydrodynamic

fields are averages of sums of single particle functions of the form

$$A = \sum_{r=1}^N a(x_r), \quad (8.1)$$

where  $x_r \longleftrightarrow (\mathbf{q}_r, \mathbf{v}_r)$  is used to denote both the position and velocity of particle  $r$ . The  $N$  particle average of such functions can be reduced to an average over the single particle phase space

$$\langle A; t \rangle = \int dx_1 a(x_1) N \int dx_2 \dots dx_N \rho(\Gamma, t) = n \int dx_1 a(x_1) f^{(1)}(x_1, t), \quad (8.2)$$

where  $f^{(1)}(x_1, t)$  is the first member of a family of reduced distribution functions obtained by integrating out some degrees of freedom

$$n^m f^{(m)}(x_1, \dots, x_m, s) \equiv \frac{N!}{(N-m)!} \int dx_{m+1} \dots dx_N \rho(\Gamma, s). \quad (8.3)$$

Clearly,  $f^{(1)}(x_1, t)$  is proportional to the exact probability density to find a particle with  $(\mathbf{q}_1, \mathbf{v}_1)$  at time  $t$ , regardless of the phase of all other particles. The representation (8.2) expresses the fact the much less information is required for such averages than is contained in the full  $N$  particle state of the system  $\rho(\Gamma, t)$ , and that it is sufficient to know the dynamics in the single particle phase space.

Equations for the dynamics in the reduced distribution functions follow from the Liouville equation by integrating it over some degrees of freedom

$$\begin{aligned} & \left( \partial_t + \sum_{i=1}^m \mathbf{v}_i \cdot \nabla_i - \sum_{i < j}^m \bar{T}(i, j) \right) f^{(m)}(x_1, \dots, x_m, t) \\ &= n \sum_{i=1}^m \int dx_{m+1} \bar{T}(i, m+1) f^{(m+1)}(x_1, \dots, x_{m+1}, t). \end{aligned} \quad (8.4)$$

The left side of this equation describes the dynamics of  $m$  particles, just as the Liouville equation for an isolated system of  $m$  particles. The right side represents the effects due to interactions with the remaining  $N - m$  particles. It describes this interaction for each of the  $m$  particles with another with  $x_{m+1}$  times the probability density that there is such a particle with this phase. The latter is the joint probability for  $m + 1$  particles. It is seen that the equation for  $f^{(m)}$  is coupled in this way to that for  $f^{(m+1)}$ . This family of equations is known as the Born, Bogoliubov, Green, Kirkwood, Yvon (BBGKY) hierarchy [10]. The simplicity of the representation (8.2) is somewhat misleading, since the many-body problem is simply transferred to the problem of solving this hierarchy.

There have been many attempts to obtain approximate solutions for  $f^{(1)}(x_1, t)$ . Most of these entail a "closure" approximation so that the first hierarchy equation becomes a closed equation for  $f^{(1)}$  alone. This is accomplished by some form of functional assumption in which it is assumed that the two particle distribution function can be expressed as a functional of the one particle distribution

$$f^{(2)}(x_1, x_1, t) \rightarrow F(x_1, x_2, t | f^{(1)}(t)) \quad (8.5)$$

If the functional form  $F(x_1, x_2, t | \cdot)$  can be discovered then the first BBGKY hierarchy becomes a *kinetic equation*

$$(\partial_t + \mathbf{v}_1 \cdot \nabla_1) f^{(1)}(x_1, t) = J(x_1, t | f^{(1)}(t)), \quad (8.6)$$

where the collision operator  $J(x_1, t | f^{(1)}(t))$  is identified as

$$J(x_1, t | f^{(1)}(t)) \equiv n \int dx_2 \bar{T}(1, 2) F(x_1, x_2, t | f^{(1)}(t)). \quad (8.7)$$

In fact, (8.5) is so general that such a construction is always possible in principle. A meaningful physical approximation requires further guidance. Bogoliubov argued [30] that in many cases there is an initial "synchronization" time after which this functional exists as a time independent functional

$$f^{(2)}(x_1, x_1, t) \rightarrow F(x_1, x_2 | f^{(1)}(t)). \quad (8.8)$$

In this case the kinetic equation is Markovian. Bogoliubov then went on to construct this functional formally as an expansion in the reduced density as a small parameter. This procedure was formalized by others via cluster expansions, which allowed a more penetrating analysis of terms in the expansion. It was found that the expansion is not uniform in time, due to an unexpected class of recollisions of particles ("rings") leading to secular contributions. A similar detailed analysis for granular systems has not yet been carried out.

Here, a formal solution to the hierarchy will be constructed for low density gases using again the reduced density as a small parameter and for the special case of inelastic hard spheres. This expansion is initiated by returning to the dimensionless form of the Liouville equation (3.40). The corresponding dimensionless form of the hierarchy is found to be

$$\left( \partial_s + \bar{\mathcal{L}}_m^*(\epsilon) \right) f^{*(m)}(x_1^*, \dots, x_m^*, s) = \sum_{i=1}^m \int dx_{m+1} \bar{T}^*(i, m+1) f^{*(m+1)}(x_1^*, \dots, x_{s+1}^*, s). \quad (8.9)$$

with the definitions

$$f^{*(m)}(x_1^*, \dots, x_m^*, s) \equiv (n\ell^3 v_h^3(t))^m f^{(m)}(x_1, \dots, x_m, t) \quad (8.10)$$

$$\bar{\mathcal{L}}_m^*(\epsilon) X \equiv \sum_{i=1}^m \left( \mathbf{v}_i^* \cdot \nabla_{\mathbf{q}_i^*} X + \frac{\zeta_h^*}{2} \nabla_{\mathbf{v}_i^*} \cdot [\mathbf{v}_i^* X] \right) - \epsilon^2 \sum_{i < j}^m \bar{T}^*(i, j) X \quad (8.11)$$

$$\begin{aligned} \bar{T}^*(i, j) &\equiv \frac{\ell}{v_h(t)} \left( \frac{\ell}{\sigma} \right)^2 \bar{T}(i, j) \\ &= \int d\hat{\sigma} \Theta(\mathbf{g}_{ij}^* \cdot \hat{\sigma}) (\mathbf{g}_{ij}^* \cdot \hat{\sigma}) [\alpha^{-2} \delta(\mathbf{q}_{ij}^* - \epsilon \hat{\sigma}) b_{ij}^{-1} - \delta(\mathbf{q}_{ij}^* + \epsilon \hat{\sigma})] \end{aligned} \quad (8.12)$$

$$\epsilon \equiv \frac{\sigma}{\ell} = n\sigma^3 \quad (8.13)$$

The length scale has been chosen to be the mean free path  $\ell \equiv 1/(n\sigma^2)$ , where  $n$  is the density. Low density is now defined by  $\epsilon \ll 1$ , i.e. the grain size is small compared to the mean free path. This suggests looking for a solution to the hierarchy as an expansion in this small parameter

$$f^{*(m)} = f_0^{*(m)} + \epsilon f_1^{*(m)} + \dots \quad (8.14)$$

It is readily shown [31] that the hierarchy is solved exactly to zeroth order in  $\epsilon$  by

$$f_0^{(m)}(x_1, \dots, x_m, s) = \prod_{i=1}^s f_0^{*(1)}(x_i, s), \quad (8.15)$$

where  $f_0^{*(1)}(x_i, s)$  is the solution to

$$(\partial_s + \mathbf{v}_1^* \cdot \nabla_{\mathbf{q}_1^*}) f_0^{*(1)}(x_1^*, s) + \frac{\zeta_{0h}^*}{2} \nabla_{\mathbf{v}_1^*} \cdot [\mathbf{v}_1^* f_0^{*(1)}(x_1^*, s)] = J_0^*(\mathbf{v}_1^* | f_0^{*(1)}(s)). \quad (8.16)$$

The operator  $J^*$  is the Boltzmann collision operator for inelastic hard spheres [10]

$$J^*(\mathbf{v}_1^* | f_0^{*(1)}(s)) = \int dx_2^* \bar{T}_0^*(1, 2) f_0^{*(1)}(x_1^*, s) f_0^{*(1)}(x_2^*, s), \quad (8.17)$$

where  $\bar{T}_0^*(1, 2)$  is  $\bar{T}^*(i, j)$  at  $\epsilon = 0$

$$\bar{T}_0^*(i, j) = \int d\hat{\sigma} \Theta(\mathbf{g}_{ij} \cdot \hat{\sigma}) (\mathbf{g}_{ij} \cdot \hat{\sigma}) \delta(\mathbf{q}_{ij}^*) [\alpha^{-2} b_{ij}^{-1} - 1]. \quad (8.18)$$

The effect of different locations of the colliding particles (contained in the Boltzmann-Bogoliubov collision operator [30]) does not contribute at this order. Finally,  $\zeta_{0h}^*$  is given by (3.31) at  $\epsilon = 0$ , which reduces to (using the symmetry of the HCS)

$$\zeta_h^* = (1 - \alpha^2) \frac{\pi}{12} \int dv_1^* dv_2^* f_{0h}^{*(1)}(v_1^*) f_{0h}^{*(1)}(v_2^*) g_{12}^{*3}, \quad (8.19)$$

where  $f_{0h}^{*(1)}$  is the stationary HCS solution to the Boltzmann equation (8.16)

$$\frac{\zeta_{0h}^*}{2} \nabla_{\mathbf{v}_i^*} \cdot \left[ \mathbf{v}_i^* f_{0h}^{*(1)}(v_1^*) \right] = J^*(v_1^* | f_{0h}^{*(1)}(s)). \quad (8.20)$$

This provides a complete description for the determination of  $f_0^{*(1)}(x_1^*, s)$  and the calculation of averages such as (8.2) at low density. It is an exceptional non-trivial result, and somewhat special to the hard sphere interactions. A similar analysis for non-singular forces leads to a collisionless mean field theory.

It is sufficient for the purposes here to stop at this point and inquire about solutions to this kinetic equation leading to the hydrodynamics appropriate for a low density gas. However, it is instructive to digress briefly for a discussion of higher order terms. These consist of two types, those that correct the single particle distribution in the product form (8.15), and those that generate correlations. One class of terms of the first type are those coming from the  $\epsilon$  dependence of  $\bar{T}^*(i, j)$  which give the "collision transfer" corrections to the Boltzmann equation. This suggests a "renormalization" of the expansion to one in powers of  $\epsilon^2$  at constant  $\bar{T}^*(i, j)$ . Then, to lowest order the above results are obtained again but with the replacement  $\bar{T}_0^*(1, 2) \rightarrow \bar{T}^*(i, j)$ . This is the Boltzmann-Bogoliubov low density kinetic theory that retains the different locations of the colliding particles. The first corrections to this theory have the form

$$f_1^{*(m)}(x_1^*, \dots, x_m^*, s) = \sum_{j=1}^m \prod_{i \neq j}^m f_0^{*(1)}(x_i^*, s) f_1^{*(1)}(x_j^*, s) + \sum_{i < j}^m \prod_{k \neq i, j}^m f_0^{*(1)}(x_k^*, s) G^*(x_i^*, x_j^*, s), \quad (8.21)$$

where the expression for  $f_1^{*(m)}$  holds for  $m \geq 2$ . Thus, the reduced distribution functions for any number of particles are determined as a sum of products of the single particle functions  $f_0^{*(1)}(x_1^*, s)$  and  $f_1^{*(1)}(x_1^*, s)$ , and pair function  $G^*(x_1^*, x_2^*, s)$ . These are determined from the set of three fundamental kinetic equations [31]

$$\begin{aligned} & (\partial_s + \mathbf{v}_1^* \cdot \nabla_{\mathbf{q}_1^*}) f_0^{*(1)}(x_1^*, s) + \frac{\zeta_{0h}^*}{2} \nabla_{\mathbf{v}_i^*} \cdot \left[ \mathbf{v}_i^* f_0^{*(1)}(x_1^*, s) \right] \\ &= \int dx_2^* \bar{T}^*(1, 2) f_0^{*(1)}(x_1^*, s) f_0^{*(1)}(x_2^*, s). \end{aligned} \quad (8.22)$$

$$(\partial_s + \mathcal{L}_1^*) f_1^{*(1)}(x_1^*, s) = \int dx_2^* \bar{T}^*(1, 2) G^*(x_1^*, x_2^*, s). \quad (8.23)$$

$$(\partial_s + \mathcal{L}_1^* + \mathcal{L}_2^*) G^*(x_1^*, x_2^*, s) = \bar{T}^*(1, 2) f_0^{*(1)}(x_1^*, s) f_0^{*(1)}(x_2^*, s) \quad (8.24)$$

The operator  $\mathcal{L}_1^*$  is defined over functions of  $x_1^*$  by (8.22)

$$\begin{aligned} \mathcal{L}_1^* h^*(x_1^*) \equiv & \mathbf{v}_1^* \cdot \nabla_{\mathbf{q}_1^*} + \frac{\zeta_{0h}^*}{2} \nabla_{\mathbf{v}_i^*} \cdot [\mathbf{v}_i^* h^*(x_1^*)] \\ & - \int dx_2^* \overline{T}^*(1, 2) \left( f_0^{*(1)}(x_1^*, s) h^*(x_2^*) + h^*(x_1^*) f_0^{*(1)}(x_2^*, s) \right). \end{aligned} \quad (8.25)$$

These low density results (8.22)-(8.24) are remarkably rich. The first equation for the single particle distribution function is given by the Boltzmann equation, as expected. The second equation provides corrections to the Boltzmann results in terms of the two particle correlations. This provides a means to understand the limitations of the Boltzmann equation. The third equation gives the dynamics of these pair correlation. They are driven by a source term which is the result of the binary collision operator acting on uncorrelated single particle distributions that are solutions to the Boltzmann equation. In more detail, it is possible to show that the solution to this pair correlation equation, together with the equation for  $f_1^{*(1)}$  give corrections to the Boltzmann equation due to correlated recollisions ("ring" collisions) among many particles. These effects dominate at long times and therefore show that the Boltzmann theory is not accurate at asymptotically long times, no matter how low the density. The third equation also gives the means to study the dynamics of pair correlations, which also are characterized by correlation recollisions. Finally, not shown is the equation for pair correlations at two different times, which also follows from this analysis [31].

### A. Hydrodynamics from Kinetic Theory

Consider now the Boltzmann kinetic equation for the one particle distribution function (8.22). The dimensionless hydrodynamic fields, scaled relative to their values in the corresponding HCS, (8.20), are

$$\begin{pmatrix} n^*(\mathbf{r}^*, s) \\ n^*(\mathbf{r}^*, s) T^*(\mathbf{r}^*, s) \\ n^*(\mathbf{r}^*, s) \mathbf{U}^*(\mathbf{r}^*, s) \end{pmatrix} = \int d\mathbf{v}^* \begin{pmatrix} 1 \\ \frac{1}{3} v^{*2} \\ \mathbf{v}^* \end{pmatrix} f^*(\mathbf{r}^*, \mathbf{v}^*, s) \quad (8.26)$$

Multiplying by (8.22) by 1,  $v^{*2}$ , and  $\mathbf{v}^*$  and integrating, successively, gives the macroscopic balance equations. They are the same as those of (4.12)-(4.14), in dimensionless form, except for expressions defining the cooling rate, heat flux, and pressure tensor. Here they

are integrals over  $f^*(x_1^*, s)$

$$\zeta^* = (1 - \alpha^2) \frac{\pi}{12T^*} \int dv_1^* dv_2^* f^*(\mathbf{r}^*, \mathbf{v}^*, s) f^*(\mathbf{r}^*, \mathbf{v}^*, s) g_{12}^{*3} \quad (8.27)$$

$$P_{ij}^* = 2 \int d\mathbf{v}^* V_i^* V_j^* f^*(\mathbf{r}^*, \mathbf{v}^*, s), \quad \mathbf{q}^* = \int d\mathbf{v}^* V^{*2} \mathbf{V}^* f^*(\mathbf{r}^*, \mathbf{v}^*, s), \quad (8.28)$$

and  $\mathbf{V}^* = \mathbf{v}^* - \mathbf{U}^*(\mathbf{r}^*, s)$ .

The conceptual discussion in the sections above showing that hydrodynamics follows from the existence of a normal state applies here as well [29]. A normal solution to the Boltzmann equation for first order in the gradients (Navier-Stokes hydrodynamics) is obtained in a way analogous to that for the Liouville equation in Section VII [32]. The solution is written as

$$f^*(\mathbf{r}^*, \mathbf{v}^*, s) = f_{\ell h}^*(V^*, \{y_\alpha^*(\mathbf{r}^*, s)\}) + \Delta(\mathbf{r}^*, \mathbf{v}^* | \{y_\alpha^*(s)\}). \quad (8.29)$$

The reference state  $f_{\ell h}^*$  is the local HCS distribution given by

$$f_{\ell h}^*(V^*, \{y_\alpha^*(\mathbf{r}^*, s)\}) = n^*(\mathbf{r}^*, s) f_h^*\left(\frac{V^*}{\sqrt{T^*(\mathbf{r}^*, s)}}\right), \quad (8.30)$$

where  $f_h^*(v^*)$  is the HCS solution given by (8.20). Because of this choice for the reference state it is found that  $\Delta(\mathbf{r}^*, \mathbf{v}^* | \{y_\alpha^*(s)\})$  is of first order in the gradients

$$\begin{aligned} (\partial_s + \mathcal{L}_{01}^*) \Delta &= -(\partial_s + \mathbf{v}^* \cdot \nabla_{\mathbf{r}^*}) f_{\ell h}^* \\ &= -\frac{\partial f_{\ell h}^*}{\partial y_\nu^*} (N_\nu^* + \delta_{2\nu} \zeta^* T^* + \mathbf{v}^* \cdot \nabla_{\mathbf{r}^*} y_\nu^*) \end{aligned} \quad (8.31)$$

The subscript 0 on  $\mathcal{L}_{01}^*$  means that the spatial gradient contribution to  $\mathcal{L}_1^*$  in (8.25) is excluded ( $\mathcal{L}_{01}^* = \mathcal{L}_1^* - \mathbf{v}^* \cdot \nabla_{\mathbf{r}^*}$ ). In the first equality, use has been made of the fact  $f_{\ell h}^*$  is related to the HCS solution by (8.30). The second term contains the hydrodynamic fluxes  $N_\nu^* + \delta_{2\nu} \zeta^* T^*$  (recall equation (5.2)) which are first order in the gradients. As in Section VII, it is essential that the reference state is an exact solution to zeroth order in the gradients to assure that  $\Delta$  is of first order

$$\Delta(\mathbf{r}^*, \mathbf{v}^* | \{y_\alpha^*(s)\}) \rightarrow \mathbf{G}_\alpha^*(s, \mathbf{V}^*, \{y_\alpha^*(\mathbf{r}^*, s)\}) \cdot \nabla^* y_\alpha^*(\mathbf{r}^*, s). \quad (8.32)$$

Substituting this form into (8.30), the analysis proceeds in a similar manner to that described for the Liouville equation in Appendix E. The details will not be given and only the result is quoted for the normal solution

$$f^*(\mathbf{V}^*, \{y_\alpha^*\}) = f_{\ell h}^*(V^*, \{y_\alpha^*\}) - \left( \lim \int_0^s ds' \left( e^{-(I\mathcal{L}_{01}^* - \Lambda^*)s'} (1 - \mathcal{P}_1^*) \Upsilon^* \right)_\nu \right) \cdot \nabla^* y_\nu^*. \quad (8.33)$$



The corresponding normal average for some property  $X(\mathbf{v})$

$$\langle X; \{y_\alpha^*\} \rangle_n^* = \langle X; \{y_\alpha^*\} \rangle_{hl}^* + \left( \int_0^\infty ds \mathbf{C}_\nu^{*X}(s; \{y_\alpha^*\}) \right) \cdot \nabla y_\nu^*, \quad (8.34)$$

$$\mathbf{C}_\nu^{*X}(s; \{y_\alpha^*\}) = - \int d\mathbf{v} X(\mathbf{v}) (1 - \mathcal{P}_1^*) \left( e^{-(I\bar{\mathcal{L}}_{01}^* - \Lambda^*)s} (1 - \mathcal{P}_1^*) \mathbf{\Upsilon}^*(\mathbf{v}) \right)_\nu. \quad (8.35)$$

These results should be compared with those of Section VII to note that they have the same form as those for the Liouville equation. The single particle projection operator now projects orthogonal to the invariants of  $(I\bar{\mathcal{L}}_{01}^* - \Lambda^*)$ , where  $\Lambda^*$  is the same matrix as in (7.29),

$$(I\bar{\mathcal{L}}_{01}^* - \Lambda^*) \Psi_\alpha = 0, \quad (8.36)$$

$$\mathcal{P}^{(1)} X(\mathbf{v}) = \Psi_\alpha(\mathbf{V}, \{y_\alpha\}) \int d\mathbf{v}_1 \tilde{A}_\beta(\mathbf{V}_1, \{y_\alpha\}) X(\mathbf{v}_1), \quad (8.37)$$

$$\Psi_\alpha(\mathbf{V}, \{y_\alpha\}) = \frac{\partial f_{\ell h}(V, \{y_\alpha\})}{\partial y_\alpha}, \quad \tilde{A}_\beta(\mathbf{V}, \{y_\alpha\}) = \begin{pmatrix} 0 \\ \frac{2}{3n^*} (V^{*2} - \frac{3}{2}T^*) \\ \frac{1}{n^*} \mathbf{V}^* \end{pmatrix}. \quad (8.38)$$

Also, the flux  $\mathbf{\Upsilon}^*(\mathbf{v})$  is generated from the HCS in much the same way

$$\begin{aligned} (1 - \mathcal{P}_1^*) \mathbf{\Upsilon}^*(\mathbf{v}) &= - (1 - \mathcal{P}_1^*) (I\bar{\mathcal{L}}_1^* - \Lambda^*) \mathbf{q} \Psi_\alpha \\ &= - (1 - \mathcal{P}_1^*) \mathbf{V} \Psi_\alpha \end{aligned} \quad (8.39)$$

The constitutive equations for Navier-Stokes hydrodynamics also are the same as those of Section VII, and follow from insertion of (8.33) into (8.27) and (8.28). The transport coefficients are of course different, due to the limitations imposed by the low density approximations. For example, the shear viscosity is now

$$\eta^*(\{y_\alpha\}) = - \lim \int_0^s ds' \int d\mathbf{v} H_{xy} e^{-(\bar{\mathcal{L}}_{01}^* - \lambda_3)s'} \Upsilon_\eta, \quad (8.40)$$

$$H_{xy} = v_x v_y, \quad \Upsilon = v_x \partial_{v_y} f_h^*(V^*) \quad (8.41)$$

This is quite similar to the general result (7.32). The first term on the right side of that result vanishes in the low density limit and does not appear here. It has been shown that the general result reduces to this obtained from kinetic theory when the correlation function there is evaluated with the same low density assumptions as applied here [33]. The details for other transport coefficients are described in [34, 35] and will not be repeated here. It is found that the results agree in detail with those obtained from the alternative

Chapman-Enskog method to construct a normal solution (properly adapted to the granular Boltzmann equation [36]). The Chapman-Enskog representation requires solution to an integral equation. This has been done approximately, using a truncated polynomial expansion for the solution (or equivalently, using the cumulant expansion approximation described for the diffusion coefficient above). The Green-Kubo representation given here provides another approach to evaluation using direct Monte Carlo simulation of the correlation function [37].

## IX. DISCUSSION

The presentation given here has addressed the origins of hydrodynamics for a granular fluid. There have been three components to the discussion: 1) an exact set of balance equations, based on the starting microscopic description - either Liouville dynamics or kinetic theory; 2) the concept of a normal state which implies constitutive equations in terms of the hydrodynamic fields, and hence a hydrodynamic description; and 3) an approximate construction of the normal solution for small local gradients, leading to the Navier-Stokes hydrodynamic equations. Only the last component entails specific limitations on the state conditions considered, with explicit neglect of higher order gradients in the fields. It is presumed that these state conditions can be controlled to assure small gradients, and then Navier-Stokes hydrodynamics would apply. Below, it will be noted that some new kinds of steady states for granular fluids preclude the control over gradients and that conditions for Navier-Stokes hydrodynamics cannot be attained in these cases. But there are many other cases, verified in both simulations and experiments, for which a Navier-Stokes order hydrodynamics is found to give an accurate description [38, 39, 40, 41]. It is worth emphasizing again that the failure of a Navier-Stokes description does not mean the absence of a hydrodynamic description, only that the constitutive equations are more complex.

Even when the gradients are small, it is expected that the hydrodynamic description will dominate all other "microscopic" excitations only on some sufficiently long time scale. Thus the characteristic hydrodynamic times should be long compared to the decay times for all other excitations. For normal fluids this is assured by the fact that the hydrodynamic fields are associated with global conserved quantities (number, energy, and momentum), whose lifetimes become infinite in the long wavelength limit, while all other characteristic times remain finite. This is not the case for granular fluids, since the energy is no longer

conserved. Instead, in the long wavelength limit there is a new characteristic time determined by homogeneous cooling,  $\zeta_h^{-1}$ . Some have argued that for this reason the energy or temperature should not be considered among the hydrodynamic fields for a granular gas. However, there are many good reasons why the temperature should remain one of the fields in the long time, long wavelength description of granular fluids. For example, consider the simplest case of a general homogeneous state. On the time scale of a few collisions it approaches the HCS for which the temperature obeys Haff's law (3.34). The latter is the exact hydrodynamic description in this case which is seen to dominate even though it has a time scale  $\zeta_h^{-1}$ . For spatially inhomogeneous states, it has been shown here that the dominant background cooling can be suppressed by the dimensionless representation. This means that the relevant approach to hydrodynamics is relative to this background state. The picture described above of each cell in the fluid rapidly approaching a local HCS due to velocity relaxation, followed by approach to spatial uniformity by fluxes between the homogeneously cooling cells is consistent with this.

A more precise study of this problem is possible within the simplifying features of the Boltzmann kinetic theory. There the response to an initial small spatial perturbation of the HCS can be studied to see if there is a dominant set of collective modes at long times and long wavelengths. For a normal fluid this is established by showing that the spectrum of the generator for dynamics in the linearized Boltzmann equation has five isolated points that are smaller in magnitude than all other spectral points, and therefore dominate at long times. These are shown to exist and to be the same as the eigenvalues of the linearized hydrodynamic equations. A similar analysis of the linearized granular Boltzmann operator has shown the existence of hydrodynamic eigenvalues in its spectrum in the long wavelength limit [35, 42]. Further progress can be made using kinetic models for this Boltzmann operator, showing that the hydrodynamic modes of the spectrum remain isolated and smallest, even for strong dissipation [42, 43]. In summary, there is very good evidence for the dominance of a hydrodynamic description for granular gases in the long time, long wavelength limit.

As with normal fluids, there are states for which the simple Navier-Stokes form for hydrodynamics does not apply because the gradients are no longer small. In the case of normal fluids steady states can generally be studied in the Navier-Stokes domain by external control of boundary conditions. For granular fluids, there are new types of steady states associated

with an autonomous balance of external constraints and the internal cooling. For example, a fluid under shear has viscous heating due to the work done on it at the boundaries. Normally this is compensated by a temperature gradient that induces a compensating heat flux to produce the steady state. However, a granular fluid can compensate for the external work done via its collisional cooling. The latter scales as  $T^{3/2}$  so any amount of work done can be accommodated by the system choosing an appropriate steady state temperature. This balance is given by the energy balance equation (4.13) whose steady state form becomes, for uniform temperature and density

$$\zeta(n, T_s)T_s = -\frac{2}{3n}P_{\alpha\beta}\partial_\alpha U_\beta. \quad (9.1)$$

This imposes a relationship of the given boundary shear, the coefficient of restitution  $\alpha$ , and the steady state temperature  $T_s$ . Any attempt to produce small gradients by decreasing the boundary shear also decreases  $T_s$  at constant  $\alpha$ . Since the dimensionless measure of small shear scales as  $T^{-1/2}$  it is found that this dimensionless shear can never be brought within the accuracy of the Navier-Stokes hydrodynamics [44]. Another example of this is a granular fluid pinned between two walls at constant temperature. The internal cooling introduces a temperature gradient toward lower temperatures between the walls. The gradients established are controlled by the cooling and cannot be made small by changing the boundary temperatures. It can be shown that the steady state temperature profile is never that of the Navier-Stokes hydrodynamic prediction [44]. Such discrepancies have been seen in recent molecular dynamics simulations [45].

These last observations justify characterizing granular fluids as "complex". Under some conditions they are well-described by the local partial differential equations of Navier-Stokes form; under others they have a rheology or complex dissipation that is not observed in normal fluids, or only for those with structural complexity. Studies to date suggest that a hydrodynamic description in its most general sense - closed equations for the hydrodynamic fields - is a reasonable expectation, although the associated constitutive equations may be complicated and state dependent. Discovery of generic constitutive equations (e.g., for shear flow) is both the challenge and opportunity posed by granular fluids.

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## APPENDIX A: HARD SPHERE DYNAMICS

### 1. Generator of Trajectories

The phase function  $A(\Gamma)$  in (3.4) is evaluated at a phase point  $\Gamma_t = \{\mathbf{q}_1(t), \dots, \mathbf{q}_N(t), \mathbf{v}_1(t), \dots, \mathbf{v}_N(t)\}$  which has evolved from its initial point at  $t = 0$ ,  $\Gamma = \{\mathbf{q}_1, \dots, \mathbf{q}_N, \mathbf{v}_1, \dots, \mathbf{v}_N\}$ . Therefore  $A(\Gamma_t)$  can be considered as a function of the initial point and time,  $A(\Gamma_t) = A(\Gamma, t)$ . The simplest example to illustrate this is a gas of non interacting particles for which  $\Gamma_t = \{\mathbf{q}_1 + \mathbf{v}_1 t, \dots, \mathbf{q}_N + \mathbf{v}_N t, \mathbf{v}_1, \dots, \mathbf{v}_N\}$ . This corresponds to free streaming of all particles at constant velocities. A phase function at time  $t$  can therefore be expressed in terms of a generator for the dynamics in the following way

$$\begin{aligned} A(\Gamma_t) &= A(\{\mathbf{q}_1 + \mathbf{v}_1 t, \dots, \mathbf{q}_N + \mathbf{v}_N t, \mathbf{v}_1, \dots, \mathbf{v}_N\}) \\ &= e^{L_0 t} A(\{\mathbf{q}_1, \dots, \mathbf{q}_N, \mathbf{v}_1, \dots, \mathbf{v}_N\}), \end{aligned} \quad (\text{A1})$$

where  $L$  is the sum of generators for translations for each particle coordinate

$$L_0 = \sum_r \mathbf{v}_r \cdot \nabla_{\mathbf{q}_r}. \quad (\text{A2})$$

In this form the dependence on  $\Gamma$  and  $t$  is made explicit.

In the presence of interactions among the particles the time dependence of the positions and velocities is more complex, but still given by a deterministic rule for evolution of the initial point. If the particle interaction is pairwise additive and due to conservative, non-singular forces  $\mathbf{F}(q_{ij})$ , then (A1) is replaced by

$$A(\Gamma_t) = e^{Lt} A(\Gamma), \quad (\text{A3})$$

where the generator  $L$

$$L = L_0 + \frac{1}{2} \sum_{r,s}^N m^{-1} \mathbf{F}(q_{ij}) \cdot (\nabla_{\mathbf{v}_i} - \nabla_{\mathbf{v}_j}). \quad (\text{A4})$$

It is easily verified that this generator changes the positions and velocities according to Hamilton's equations ( $L$  is the linear operator representing the Poisson bracket of its operand with the Hamiltonian for the system). Generalization to include non-singular, non-conservative forces is straightforward.

Hard sphere dynamics is also represented by a rule for evolution of the initial phase point: particles freely stream until one pair is at contact. At that time the velocities of that pair are changed according to a specified rule (e.g., that of (3.2)) constrained to conserve total momentum for the pair. Subsequently, all particles freely stream again until another pair is at contact, when the corresponding velocity transformation of that pair is introduced. The generator for this process cannot be represented simply as in (A4) using the corresponding singular force. To discover the correct form [21], assume the first collision is between particles 1 and 2, and let  $\tau_1(\mathbf{q}_{12}, \mathbf{g}_{12})$  denote the time at which it occurs as a function of the initial separation and relative velocity. Therefore, the time evolution of any phase function  $A(\Gamma)$  can be given compactly by

$$A(\Gamma_t) = (1 - \Theta(t - \tau_1)) A(\Gamma_t) + \Theta(t - \tau_1) A(\Gamma_t) + \dots \quad (\text{A5})$$

where  $\Theta$  is the Heaviside step function,

$$\Theta(x) = \begin{pmatrix} 1, & x \geq 0 \\ 0, & x < 0 \end{pmatrix}.$$

The dots in (A5) denote contributions that arise only on the time scale of the third and later collisions. The first term on the right side of the first line contributes only for times before the first collision, so that  $\mathbf{q}_{1,2}(t) = \mathbf{q}_{1,2} + \mathbf{v}_{1,2}t$ ,  $\mathbf{v}_{1,2}(t) = \mathbf{v}_{1,2}$ . The second term contributes only after that collision, so  $\mathbf{q}_{1,2}(t) = \mathbf{q}_{1,2} + \mathbf{v}_{1,2}\tau_1 + \mathbf{v}'_{1,2}(t - \tau_1)$ ,  $\mathbf{v}_{1,2}(t) = \mathbf{v}'_{1,2}$ . The prime indicates that the velocities of the colliding pair have been changed for  $t > \tau_1$  according to the collision rule (3.2)

$$\mathbf{v}'_1 = \mathbf{v}_1 - \frac{1}{2}(1 + \alpha)(\hat{\mathbf{q}}_{12} \cdot \mathbf{g}_{12})\hat{\mathbf{q}}_{12}, \quad \mathbf{v}'_2 = \mathbf{v}_2 + \frac{1}{2}(1 + \alpha)(\hat{\mathbf{q}}_{12} \cdot \mathbf{g}_{12})\hat{\mathbf{q}}_{12}. \quad (\text{A6})$$

This distinction between  $\Gamma = \{\mathbf{q}_1(t), \dots, \mathbf{q}_N(t), \mathbf{v}_1(t), \dots, \mathbf{v}_N(t)\}$  for  $t < \tau_1$  and  $t \geq \tau_1$  reflects the discontinuity in the velocity at  $t = \tau_1$ .

Differentiation of (A6) with respect to time gives

$$\partial_t A(\Gamma_t) = (\mathbf{v}_1(t) \cdot \nabla_{\mathbf{q}_1(t)} + \mathbf{v}_2(t) \cdot \nabla_{\mathbf{q}_2(t)}) A(\Gamma_t) + \delta(t - \tau_1) (\Delta A(\Gamma_{\tau_1}) - A(\Gamma_{\tau_1 - \epsilon})) + \dots \quad (\text{A7})$$

The first term is defined for times before and after the collision, with appropriate changes in  $\mathbf{q}_{1,2}(t)$  and  $\mathbf{v}_{1,2}(t)$  as given above. The second term occurs only at the time of the collision and is proportional to the discontinuity in  $\Delta A(\Gamma_{\tau_1}) = \lim_{\epsilon \rightarrow 0} (A(\Gamma_{\tau_1}) - A(\Gamma_{\tau_1 - \epsilon}))$  due to the instantaneous change in the velocities of the colliding pair. This can be represented by a substitution operator  $b_{12}(\mathbf{g}_{12}(\tau_1))$  as in (3.9), but here defined for functions of the position and velocity at time  $\tau_1$

$$\Delta A(\Gamma_{\tau_1}) = (b_{12}(\mathbf{g}_{12}(\tau_1)) - 1) A(\Gamma_{\tau_1 - \epsilon}). \quad (\text{A8})$$

Note that  $b_{12}(\mathbf{g}_{12}(\tau))$  changes  $\mathbf{v}_{1,2}(t)$  at constant  $\mathbf{q}_{1,2}(t)$ . The time dependence of the delta function can be expressed through  $\mathbf{q}_{12}(t) - \mathbf{q}_{12}(\tau_1) = \mathbf{g}_{12}(t - \tau_1)$ , where  $\mathbf{g}_{12}$  is the relative velocity before the collision. By definition of the hard sphere collision  $\mathbf{q}_{12}(\tau_1) = \boldsymbol{\sigma}$  is a vector of length  $\sigma$  implying contact between the two particles. This can occur only if the particles are directed toward each other, i.e. for  $\hat{\boldsymbol{\sigma}} \cdot \mathbf{g}_{12} < 0$ . Thus the delta function in time can be written in terms of a delta function for position

$$\begin{aligned} \delta(t - \tau_1) &= \Theta(-\hat{\boldsymbol{\sigma}} \cdot \mathbf{g}_{12}) \delta\left(\frac{\hat{\boldsymbol{\sigma}} \cdot (\mathbf{q}_{12}(t) - \mathbf{q}_{12}(\tau_1))}{|\hat{\boldsymbol{\sigma}} \cdot \mathbf{g}_{12}|}\right) \\ &= \Theta(-\hat{\boldsymbol{\sigma}} \cdot \mathbf{g}_{12}) |\hat{\boldsymbol{\sigma}} \cdot \mathbf{g}_{12}| \delta(q_{12}(t) - \sigma). \end{aligned} \quad (\text{A9})$$

Hence (A11) takes the form

$$\begin{aligned} \partial_t A(\Gamma_t) &= (\mathbf{v}_1(t) \cdot \nabla_{\mathbf{q}_1(t)} + \mathbf{v}_2(t) \cdot \nabla_{\mathbf{q}_2(t)}) A(\Gamma_t) \\ &\quad + \delta(q_{12}(t) - \sigma) \Theta(-\hat{\boldsymbol{\sigma}} \cdot \mathbf{g}_{12}(\tau_1)) |\hat{\boldsymbol{\sigma}} \cdot \mathbf{g}_{12}(\tau_1)| \\ &\quad \times (b_{12}(\mathbf{g}_{12}(\tau_1)) - 1) A(\Gamma(\tau_1)) + \dots \end{aligned} \quad (\text{A10})$$

Since the delta function enforces  $t = \tau_1$  the latter can be expressed equivalently as  $t$  in the second term. With the representation (A3) the generator of trajectories  $L$  is identified as

$$\begin{aligned} L &= \mathbf{v}_1 \cdot \nabla_{\mathbf{q}_1} + \mathbf{v}_2 \cdot \nabla_{\mathbf{q}_2} + T(1, 2) + \dots \\ &= L_0 + \frac{1}{2} \sum_{r,s}^N T(r, s) \end{aligned} \quad (\text{A11})$$

with the binary collision operator  $T(r, s)$  given by

$$T(r, s) = \delta(q_{rs} - \sigma) \Theta(-\hat{\sigma}_{rs} \cdot \mathbf{g}_{rs}) |\hat{\sigma}_{rs} \cdot \mathbf{g}_{rs}| (b_{rs} - 1). \quad (\text{A12})$$

The second line of (A11) extends the analysis to longer times where there is sufficient time for many collisions.

## 2. Two adjoint generators

Next, consider the generator  $\bar{L}$  defined in (3.10). This can be identified from

$$\begin{aligned} \int d\Gamma A(\Gamma) \bar{L} \rho(\Gamma) &\equiv - \int d\Gamma (LA(\Gamma)) \rho(\Gamma) \\ &= - \sum_{r=1}^N \int d\Gamma \rho(\Gamma) (\mathbf{v}_r \cdot \nabla_{\mathbf{q}_r} A(\Gamma)) - \frac{1}{2} \sum_{r,s}^N \int d\Gamma \rho(\Gamma) \delta(q_{rs} - \sigma) \\ &\quad \times \Theta(-\hat{\sigma}_{rs} \cdot \mathbf{g}_{rs}) |\hat{\sigma}_{rs} \cdot \mathbf{g}_{rs}| (b_{rs} - 1) A(\Gamma). \end{aligned} \quad (\text{A13})$$

Define the inverse of  $b_{rs}$  by  $b_{rs}^{-1} b_{rs} = b_{rs} b_{rs}^{-1} = 1$ ,

$$b_{rs}^{-1} \mathbf{g}_{rs} \equiv \mathbf{g}_{rs}'' = \mathbf{g}_{rs} - (1 + \alpha) \alpha^{-1} (\hat{\sigma}_{rs} \cdot \mathbf{g}_{rs}) \hat{\sigma}_{rs}. \quad (\text{A14})$$

A useful identity is given by

$$\int d\Gamma X(\Gamma) b_{rs} Y(\Gamma) = \int d\Gamma \alpha^{-1} X(b_{rs}^{-1} \Gamma) Y(\Gamma). \quad (\text{A15})$$

This follows by changing integration variables from  $(\mathbf{v}_r, \mathbf{v}_s)$  to  $(b_{rs} \mathbf{v}_r, b_{rs} \mathbf{v}_s)$ . The factor  $\alpha^{-1}$  is the Jacobian for this change of variables. Also

$$b_{rs}^{-1} (\hat{\sigma}_{rs} \cdot \mathbf{g}_{rs}) = -\alpha^{-1} \hat{\sigma}_{rs} \cdot \mathbf{g}_{rs}. \quad (\text{A16})$$

With these results (A13) becomes

$$\begin{aligned} \int d\Gamma A(\Gamma) \bar{L} \rho(\Gamma) &= \sum_{i=1}^N \left( \int d\Gamma \rho(\Gamma) (\mathbf{v}_i \cdot \nabla_{\mathbf{q}_i} A(\Gamma)) + \int_S d\hat{\mathbf{q}}_r \cdot \int d\mathbf{v}_r d\Gamma_{s \neq r} (\mathbf{v}_r \rho(\Gamma) A(\Gamma)) \right) \\ &\quad + \frac{1}{2} \sum_{r,s} \int d\Gamma A(\Gamma) \delta(q_{rs} - \sigma) |\hat{\sigma}_{rs} \cdot \mathbf{g}_{rs}| \\ &\quad \times \left( \Theta(\hat{\sigma}_{rs} \cdot \mathbf{g}_{rs}) \alpha^{-2} b_{rs}^{-1} - \Theta(-\hat{\sigma}_{rs} \cdot \mathbf{g}_{rs}) \right) \rho(\Gamma). \end{aligned} \quad (\text{A17})$$

An integration by parts has been performed and the formal adjoint Liouville operator is identified as

$$\bar{L} = L_0 - \frac{1}{2} \sum_{r,s}^N \bar{T}(r, s), \quad (\text{A18})$$



where, the new binary collision operator is

$$\overline{T}(r, s) = \delta(q_{rs} - \sigma) |\mathbf{g}_{rs} \cdot \hat{\mathbf{q}}_{rs}| \left( \Theta(\mathbf{q}_{rs} \cdot \mathbf{g}_{rs}) \alpha^{-2} b_{rs}^{-1} - \Theta(-\mathbf{q}_{rs} \cdot \mathbf{g}_{rs}) \right). \quad (\text{A19})$$

A second adjoint generator can be interpreted as that for reversed dynamics [12]. It is defined by (3.14)

$$e^{-t\overline{L}}(\rho(\Gamma)B(\Gamma)) = \left( e^{-t\overline{L}}\rho(\Gamma) \right) (e^{-tL_-}B(\Gamma)), \quad (\text{A20})$$

or equivalently

$$\overline{L}(\rho(\Gamma)B(\Gamma)) = (\overline{L}\rho(\Gamma)) B(\Gamma) + \rho(\Gamma) (L_-B(\Gamma)), \quad (\text{A21})$$

The distributive property of (A22) is clearly satisfied by  $L_0$ , so  $L_-$  can be written in the form

$$L_- \equiv L_0 - \frac{1}{2} \sum_{r,s=1}^N T_-(r, s). \quad (\text{A22})$$

The new binary operator  $T_-(i, j)$  is identified from the corresponding condition

$$\begin{aligned} \rho(\Gamma)T_-(r, s)B(\Gamma) &= \overline{T}(r, s) (\rho(\Gamma)B(\Gamma)) - (\overline{T}(r, s)\rho(\Gamma)) B(\Gamma) \\ &= \delta(q_{rs} - \sigma) \alpha^{-1} b_{rs}^{-1} |\mathbf{g}_{rs} \cdot \hat{\mathbf{q}}_{rs}| \Theta(-\hat{\mathbf{g}}_{rs} \cdot \hat{\mathbf{q}}_{rs}) (\rho(\Gamma)B(\Gamma)) \\ &\quad - B(\Gamma) \delta(q_{rs} - \sigma) \alpha^{-1} b_{rs}^{-1} |\mathbf{g}_{rs} \cdot \hat{\mathbf{q}}_{rs}| \Theta(-\hat{\mathbf{g}}_{rs} \cdot \hat{\mathbf{q}}_{rs}) \rho(\Gamma). \\ &= [\delta(q_{rs} - \sigma) \alpha^{-1} b_{rs}^{-1} |\mathbf{g}_{rs} \cdot \hat{\mathbf{q}}_{rs}| \Theta(-\hat{\mathbf{g}}_{rs} \cdot \hat{\mathbf{q}}_{rs}) \rho(\Gamma)] (b_{rs}^{-1} - 1) B(\Gamma) \\ &= \rho(\Gamma) \delta(q_{rs} - \sigma) |\mathbf{g}_{rs} \cdot \hat{\mathbf{q}}_{rs}| \Theta(\hat{\mathbf{g}}_{rs} \cdot \hat{\mathbf{q}}_{rs}) (b_{rs}^{-1} - 1) B(\Gamma). \end{aligned} \quad (\text{A23})$$

The last equality follows from a boundary condition for hard particles at contact

$$\delta(q_{rs} - \sigma) \alpha^{-1} b_{rs}^{-1} |\mathbf{g}_{rs} \cdot \hat{\mathbf{q}}_{rs}| \Theta(-\hat{\mathbf{g}}_{rs} \cdot \hat{\mathbf{q}}_{rs}) \rho(\Gamma) = \delta(q_{rs} - \sigma) |\mathbf{g}_{rs} \cdot \hat{\mathbf{q}}_{rs}| \Theta(\hat{\mathbf{g}}_{rs} \cdot \hat{\mathbf{q}}_{rs}) \rho(\Gamma). \quad (\text{A24})$$

This can be understood from the fact that the flux of particles moving towards each other at contact must equal the flux of particles separating at contact. Since the velocities of the former and latter are, respectively,  $\mathbf{g}'_{ij} = b_{ij}^{-1} \mathbf{g}_{ij}$  and  $\mathbf{g}_{ij}$ , this gives [46]

$$\delta(q_{rs} - \sigma) |\mathbf{g}'_{rs} \cdot \hat{\mathbf{q}}_{rs}| \Theta(-\mathbf{g}'_{rs} \cdot \hat{\mathbf{q}}_{rs}) \rho(\Gamma') d\Gamma' = \delta(q_{rs} - \sigma) |\mathbf{g}_{rs} \cdot \hat{\mathbf{q}}_{rs}| \Theta(\hat{\mathbf{g}}_{rs} \cdot \hat{\mathbf{q}}_{rs}) \rho(\Gamma) d\Gamma. \quad (\text{A25})$$

This result implies (A24). The form for  $T_-(i, j)$  is then identified from (A23) as

$$T_-(r, s) = \delta(q_{rs} - \sigma) |\mathbf{g}_{rs} \cdot \hat{\mathbf{q}}_{rs}| \Theta(\hat{\mathbf{g}}_{rs} \cdot \hat{\mathbf{q}}_{rs}) (b_{rs}^{-1} - 1) \quad (\text{A26})$$

## APPENDIX B: BALANCE EQUATIONS AND FLUXES

In this appendix, the forms of the fluxes and sources associated with the local number density  $\hat{n}$ , energy density  $\hat{e}$ , and momentum density  $\hat{\mathbf{g}}$  are identified from the microscopic balance equations associated with these densities. Consider first the case for phase functions of the form

$$A(\mathbf{r}, t) = e^{Lt} A(\mathbf{r}), \quad A(\mathbf{r}) = \sum_{s=1}^N a(\mathbf{v}_s) \delta(\mathbf{r} - \mathbf{q}_s). \quad (\text{B1})$$

Its forward time evolution is

$$(\partial_t - L) A(\mathbf{r}, t) = 0 \quad (\text{B2})$$

The action of the Liouville operator is

$$\begin{aligned} LA(\mathbf{r}) &= -\nabla_{\mathbf{r}} \cdot \sum_{s=1}^N \mathbf{v}_s a(\mathbf{v}_s) \delta(\mathbf{r} - \mathbf{q}_s) \\ &\quad + \frac{1}{2} \sum_{r,s} T(r, s) (\delta(\mathbf{r} - \mathbf{q}_r) a(\mathbf{v}_r) + \delta(\mathbf{r} - \mathbf{q}_s) a(\mathbf{v}_s)) \end{aligned} \quad (\text{B3})$$

Next, use the identity

$$\begin{aligned} \delta(\mathbf{r} - \mathbf{q}_r) &= \delta(\mathbf{r} - \mathbf{q}_s) + \int_0^1 d\gamma \frac{\partial}{\partial \gamma} \delta(\mathbf{r} - \mathbf{q}_s + \gamma \mathbf{q}_{sr}) \\ &= \delta(\mathbf{r} - \mathbf{q}_s) + \nabla_{\mathbf{r}_\beta} \cdot \int_0^1 d\gamma \delta(\mathbf{r} - \mathbf{q}_s + \gamma \mathbf{q}_{sr}) \mathbf{q}_{sr}, \end{aligned} \quad (\text{B4})$$

to obtain the microscopic balance equation for  $A(\mathbf{r}, t)$

$$\partial_t A(\mathbf{r}, t) + \nabla_{\mathbf{r}} \cdot \mathbf{B}(\mathbf{r}, t) = S(\mathbf{r}). \quad (\text{B5})$$

The flux  $\mathbf{B}(\mathbf{r}, t)$  is identified as

$$\mathbf{B}(\mathbf{r}) = \sum_{k=1}^N \mathbf{v}_k a(\mathbf{v}_k) \delta(\mathbf{r} - \mathbf{q}_k) - \frac{1}{2} \int_0^1 d\gamma \sum_{r,s} \delta(\mathbf{r} - \mathbf{q}_r + \gamma \mathbf{q}_{rs}) \mathbf{q}_{rs} T(r, s) a(\mathbf{v}_s). \quad (\text{B6})$$

The first term on the right side is the "kinetic" contribution due to the kinetic motion of the particles, while the second term is the "collisional transfer" part of the flux that requires no motion. The source term in the balance equation is

$$S(\mathbf{r}) = \frac{1}{2} \sum_{r=1}^N \sum_{j \neq s}^N \delta(\mathbf{r} - \mathbf{q}_r) T(r, s) (a(\mathbf{v}_r) + a(\mathbf{v}_s)) \quad (\text{B7})$$

It vanishes for any two particle "collisional invariant"  $a(\mathbf{v}_s) + a(\mathbf{v}_r)$  which is the same before and after a binary collision. For elastic collisions or conservative forces these are given by  $a(\mathbf{v}_s) = 1, \mathbf{v}, v^2$ .

Consider now the local microscopic number, energy, and momentum densities defined by

$$\hat{n} = \sum_{s=1}^N \delta(\mathbf{r} - \mathbf{q}_s), \quad \hat{e} = \sum_{s=1}^N \frac{1}{2} m \mathbf{v}_s^2 \delta(\mathbf{r} - \mathbf{q}_s), \quad \hat{\mathbf{g}} = \sum_{s=1}^N m \mathbf{v}_s \delta(\mathbf{r} - \mathbf{q}_s). \quad (\text{B8})$$

The microscopic balance equations become

$$\partial_t \hat{n}(\mathbf{r}, t) + m^{-1} \nabla_{\mathbf{r}} \cdot \hat{\mathbf{g}}(\mathbf{r}, t) = 0 \quad (\text{B9})$$

$$\partial_t \hat{e}(\mathbf{r}, t) + \nabla_{\mathbf{r}} \cdot \mathbf{s}(\mathbf{r}, t) = w(\mathbf{r}, t) \quad (\text{B10})$$

$$\partial_t \hat{g}_{\alpha}(\mathbf{r}, t) + \nabla_{\mathbf{r}_{\beta}} h_{\alpha\beta}(\mathbf{r}, t) = 0 \quad (\text{B11})$$

The absence of sources on the right sides of (B9) and (B11) occurs since 1 and  $\mathbf{v}$  are still summational invariants for inelastic collisions. The loss function in the energy equation is

$$\begin{aligned} w(\mathbf{r}) &= \frac{1}{2} \sum_{r,s}^N \delta(\mathbf{r} - \mathbf{q}_i) T(r, s) \left( \frac{1}{2} m v_r^2 + \frac{1}{2} m v_s^2 \right) \\ &= \frac{1}{2} \sum_{r,s}^N \delta(\mathbf{r} - \mathbf{q}_i) T(r, s) \frac{1}{4} m g_{rs}^2. \end{aligned} \quad (\text{B12})$$

The second equality follows from the fact that the center of mass energy is conserved, by momentum conservation. The energy and momentum fluxes are

$$\mathbf{s}(\mathbf{r}) = \sum_{s=1}^N \mathbf{v}_s \frac{1}{2} m \mathbf{v}_s^2 \delta(\mathbf{r} - \mathbf{q}_s) - \frac{1}{2} \int_0^1 d\gamma \sum_{r,s}^N \delta(\mathbf{r} - \mathbf{q}_r + \gamma \mathbf{q}_{rs}) \mathbf{q}_{rs} T(r, s) \frac{1}{2} m \mathbf{v}_s^2. \quad (\text{B13})$$

$$h_{\alpha\beta}(\mathbf{r}) = \sum_{s=1}^N m v_{s\alpha} v_{s\beta} \delta(\mathbf{r} - \mathbf{q}_r) - \frac{1}{2} \int_0^1 d\gamma \sum_{r,s}^N \delta(\mathbf{r} - \mathbf{q}_r + \gamma \mathbf{q}_{rs}) q_{rs\alpha} T(r, s) m v_{s\beta}. \quad (\text{B14})$$

### 1. Time reversed dynamics

Now consider the same phase function as in (B1) except for the reversed trajectory (still with  $t \geq 0$ )

$$(-\partial_t - L_-) A(\mathbf{r}, -t) = 0, \quad A(\mathbf{r}, -t) = e^{-L_- t} A(\mathbf{r}). \quad (\text{B15})$$

$$L_- = \sum_{s=1}^N \mathbf{v}_s \cdot \nabla_{\mathbf{q}_s} - \frac{1}{2} \sum_{r,s}^N T_-(r, s) \quad (\text{B16})$$

The derivation of balance equations for the backward dynamics is similar to that above with the result

$$-\partial_t A(\mathbf{r}, -t) + \nabla_{\mathbf{r}} \cdot \mathbf{B}_-(\mathbf{r}, -t) = S_-(\mathbf{r}). \quad (\text{B17})$$

The flux  $\mathbf{B}_-(\mathbf{r})$  is

$$\mathbf{B}(\mathbf{r}) = \sum_{s=1}^N \mathbf{v}_s a(\mathbf{v}_s) \delta(\mathbf{r} - \mathbf{q}_s) - \frac{1}{2} \int_0^1 d\gamma \sum_{r,s}^N \delta(\mathbf{r} - \mathbf{q}_r + \gamma \mathbf{q}_{rs}) \mathbf{q}_{rs} T_-(r, s) a(\mathbf{v}_s), \quad (\text{B18})$$

and the source  $S_-(\mathbf{r})$  is

$$S_-(\mathbf{r}) = -\frac{1}{2} \sum_{s=1}^N \delta(\mathbf{r} - \mathbf{q}_s) \sum_{r,s}^N T_-(r, s) (a(\mathbf{v}_r) + a(\mathbf{v}_s)). \quad (\text{B19})$$

Interestingly, the fluxes and sources for the forward and backward balance equations are not the same due to the differences between  $T(r, s)$  and  $T_-(r, s)$ . This is a peculiarity of hard spheres for both normal and granular fluids. It occurs for non-singular, non-conservative dynamics as well.

The corresponding microscopic balance equations for reversed dynamics are

$$-\frac{\partial \hat{n}(\mathbf{r}, -t)}{\partial t} + m^{-1} \nabla_{\mathbf{r}} \cdot \hat{\mathbf{g}}(\mathbf{r}, -t) = 0 \quad (\text{B20})$$

$$-\frac{\partial \hat{e}(\mathbf{r}, -t)}{\partial t} + \nabla_{\mathbf{r}} \cdot \mathbf{s}_-(\mathbf{r}, -t) = w_-(\mathbf{r}, -t) \quad (\text{B21})$$

$$-\frac{\partial \hat{g}_\alpha(\mathbf{r}, -t)}{\partial t} + \nabla_{\mathbf{r}_\beta} h_{-\alpha\beta}(\mathbf{r}, -t) = 0 \quad (\text{B22})$$

$$w_-(\mathbf{r}) = -\frac{1}{2} \sum_{r,s}^N \delta(\mathbf{r} - \mathbf{q}_r) T_-(r, s) \left( \frac{1}{2} m \mathbf{v}_r^2 + \frac{1}{2} m \mathbf{v}_s^2 \right). \quad (\text{B23})$$

The energy and momentum fluxes are

$$\mathbf{s}_-(\mathbf{r}) = \sum_s^N \mathbf{v}_s \frac{1}{2} m \mathbf{v}_s^2 \delta(\mathbf{r} - \mathbf{q}_s) + \frac{1}{2} \int_0^1 d\gamma \sum_{r,s}^N \delta(\mathbf{r} - \mathbf{q}_r + \gamma \mathbf{q}_{rs}) \mathbf{q}_{rs} T_-(r, s) \frac{1}{2} m \mathbf{v}_s^2. \quad (\text{B24})$$

$$h_{-\alpha\beta}(\mathbf{r}) = \sum_{s=1}^N m v_{s\alpha} v_{s\beta} \delta(\mathbf{r} - \mathbf{q}_s) + \frac{1}{2} \int_0^1 d\gamma \sum_{r,s}^N \delta(\mathbf{r} - \mathbf{q}_r + \gamma \mathbf{q}_{rs}) q_{rs\alpha} T_-(r, s) m v_{s\beta}. \quad (\text{B25})$$

Note that the fluxes are not the same as those for the forward time conservation laws, (B13) and (B14), because of the differences between the binary collision operators  $T(r, s)$  and  $T_-(r, s)$ . This observation is not purely of academic interest, as both sets of fluxes occur in the Green-Kubo expressions for transport coefficients for a normal fluid (see for example (7.37)).

## APPENDIX C: LOCAL REST FRAME TRANSFORMATION

The microscopic densities and fluxes can be represented in terms of contributions from local convective flow plus their values in the local rest frame. This is accomplished by a partial Galilean transformation on all velocities,  $\mathbf{v}'_s = \mathbf{v}_s - \mathbf{U}(\mathbf{r}, t)$ , where  $\mathbf{U}(\mathbf{r}, t)$  is the macroscopic flow field defined by Eq. (4.6) and the point  $\mathbf{r}$  is the same as that of the local property being considered. A straightforward calculation for the densities gives the results  $\hat{n}(\mathbf{r}) = \hat{n}'(\mathbf{r})$ ,  $l(\mathbf{r}) = l'(\mathbf{r})$  and

$$\hat{e}(\mathbf{r}) = \hat{e}'(\mathbf{r}) + \hat{\mathbf{g}}'(\mathbf{r}) \cdot \mathbf{U}(\mathbf{r}, t) + \frac{1}{2} m \hat{n}(\mathbf{r}) U^2(\mathbf{r}, t), \quad \hat{\mathbf{g}}(\mathbf{r}) = \hat{\mathbf{g}}'(\mathbf{r}) + m \hat{n}(\mathbf{r}) \mathbf{U}(\mathbf{r}, t). \quad (\text{C1})$$

A prime on a phase function indicates that same function evaluated at  $\mathbf{v}_s \rightarrow \mathbf{v}'_s$ . The energy and momentum fluxes transform according to

$$\begin{aligned} \mathbf{s}(\mathbf{r}) = & \mathbf{s}'(\mathbf{r}) + \mathbf{U}(\mathbf{r}, t) \left( \hat{e}'(\mathbf{r}) + \hat{\mathbf{g}}'(\mathbf{r}) \cdot \mathbf{U}(\mathbf{r}, t) + \frac{1}{2} m \hat{n}'(\mathbf{r}) U^2(\mathbf{r}, t) \right) \\ & + \frac{1}{2} \hat{\mathbf{g}}'(\mathbf{r}) U^2(\mathbf{r}, t) + h'_{\alpha\beta}(\mathbf{r}) \end{aligned} \quad (\text{C2})$$

$$h_{\alpha\beta}(\mathbf{r}) = h'_{\alpha\beta}(\mathbf{r}) + \hat{g}'_{\alpha}(\mathbf{r}) U_{\beta}(\mathbf{r}, t) + \hat{g}'_{\beta}(\mathbf{r}) U_{\alpha}(\mathbf{r}, t) + m \hat{n}'(\mathbf{r}) U_{\alpha}(\mathbf{r}, t) U_{\beta}(\mathbf{r}, t) \quad (\text{C3})$$

The averages of these are then  $n(\mathbf{r}, t) = n'(\mathbf{r}, t)$ ,  $\langle w(\mathbf{r}); t \rangle = \langle w'(\mathbf{r}); t \rangle$  and

$$e(\mathbf{r}, t) = e'(\mathbf{r}, t) + \frac{1}{2} m n(\mathbf{r}, t) U^2(\mathbf{r}, t), \quad \mathbf{g}(\mathbf{r}, t) = m n(\mathbf{r}, t) \mathbf{U}(\mathbf{r}, t). \quad (\text{C4})$$

$$\langle \mathbf{s}(\mathbf{r}); t \rangle = \langle \mathbf{s}'(\mathbf{r}); t \rangle + \mathbf{U}(\mathbf{r}, t) \left( e'(\mathbf{r}, t) + \frac{1}{2} m n(\mathbf{r}, t) U^2(\mathbf{r}, t) \right) + \langle h'_{\alpha\beta}(\mathbf{r}); t \rangle \quad (\text{C5})$$

## APPENDIX D: LOCAL HOMOGENEOUS COOLING STATE

The HCS solution to the Liouville equation corresponds to spatially constant hydrodynamic fields. The *local* HCS is a reference state distribution that is not a solution to the Liouville equation but approximates the true nonequilibrium normal solution. Physically, it represents a partitioning of the system into cells such that each cell is in a HCS at its own values for the fields. These values are chosen to be same as the exact values for the nonequilibrium state. This condition is expressed in (6.2). Recall that the HCS distribution has the scaling property expressed by (3.21)

$$\rho_h(\Gamma; t) = (l v_h(t))^{-Nd} \rho_h^* \left( \left\{ \frac{\mathbf{q}_{rs}}{l}, \frac{\mathbf{v}_r - \mathbf{U}_h}{v_h(t)} \right\}, n_h l^3 \right), \quad v_h(t) = \sqrt{2T_h(t)/m} \quad (\text{D1})$$

This suggests that the local HCS distribution should be defined as

$$\rho_{\ell h}(\Gamma, \{y_\alpha\}) \equiv \prod_{s=1}^N (lv(\mathbf{q}_s, t))^{-3} \rho_h^* \left( \left\{ \frac{\mathbf{q}_{rs}}{l}, \frac{\mathbf{v}_r - \mathbf{U}(\mathbf{q}_r, t)}{v(\mathbf{q}_r, t)} \right\}, n(\mathbf{q}_r, t) l^3 \right), \quad (\text{D2})$$

$$v(\mathbf{q}_r, t) = \sqrt{2T(\mathbf{q}_r, t)/m}. \quad (\text{D3})$$

The dimensionless function  $\rho_h^*$  has its arguments changed to reflect the fact that the hydrodynamic fields at the positions of each particle can be different. Thus translational invariance is broken only by the spatial dependence of the hydrodynamic fields. It is verified that (3.21) is satisfied, and clearly  $\rho_{\ell h} \rightarrow \rho_h$  if the value of the fields is the same everywhere. The stronger requirements in (6.3) are also satisfied. To illustrate, let the reference value for the fields be evaluated at a chosen point  $\mathbf{r}$  and write  $y_\alpha(\mathbf{q}_r, t) = y_\alpha(\mathbf{r}, t) + \delta y_\alpha(\mathbf{q}_r, t)$ . Then direct calculation gives

$$\int d\mathbf{r}' \frac{\delta \rho_{h\ell}(\Gamma | \{y_\beta\})}{\delta U_i(\mathbf{r}', t)} \Big|_{\delta y=0} = \frac{\partial \rho_h}{\partial U_i(\mathbf{r}, t)}. \quad (\text{D4})$$

In the same way higher functional derivatives have similar properties

$$\int d\mathbf{r}' d\mathbf{r}'' \frac{\delta \rho_{h\ell}(\Gamma | \{y_{0\beta} + \delta y_\beta\})}{\delta U_i(\mathbf{r}', t) \delta U_j(\mathbf{r}'', t)} \Big|_{\delta y=0} = \frac{\partial^2 \rho_h}{\partial U_i(\mathbf{r}, t) \partial U_j(\mathbf{r}, t)}. \quad (\text{D5})$$

These requirements exclude other choices for  $\rho_{\ell h}$  that are simply perturbations of  $\rho_h$ . The essential role of (D4) is demonstrated in the next appendix.

The modified scaling of  $\rho_{h\ell}(\Gamma, \{y_\alpha\})$  provides alternative forms for the functional derivatives with respect to temperature and velocity fields. For example,

$$\begin{aligned} \frac{\delta \rho_{h\ell}(\Gamma | \{y_\beta\})}{\delta T(\mathbf{r}', t)} \Big|_{\delta y=0} &= - \sum_{s=1}^N \frac{\delta \ln v(\mathbf{q}_s, t)}{\delta T(\mathbf{r}', t)} \nabla_{\mathbf{v}_s} \cdot (\mathbf{v}_s - \mathbf{U}(\mathbf{q}_s, t)) \rho_h(\{y_\beta(\mathbf{r}, t)\}) \\ &= - \frac{1}{2T(\mathbf{r}', t)} \sum_{s=1}^N \delta(\mathbf{q}_s - \mathbf{r}') \nabla_{\mathbf{v}_s} \cdot (\mathbf{v}_s - \mathbf{U}(\mathbf{r}', t)) \rho_h(\{y_\beta(\mathbf{r}, t)\}) \end{aligned} \quad (\text{D6})$$

Similarly, the corresponding velocity derivative can be written

$$\frac{\delta \rho_{h\ell}(\Gamma | \{y_\beta\})}{\delta U_i(\mathbf{r}', t)} \Big|_{\delta y=0} = - \sum_{s=1}^N \delta(\mathbf{q}_s - \mathbf{r}') \frac{\partial \rho_h(\{y_\beta(\mathbf{r}, t)\})}{\partial v_{si}} \quad (\text{D7})$$

These functional derivatives are therefore phase space densities derived from derivatives of  $\rho_h$  with respect to the density.

As stated above, the local HCS distribution is not a solution to the Liouville equation. Instead, it differs from a solution by terms proportional to gradients in the hydrodynamic fields.

## APPENDIX E: SOLUTION TO THE LIOUVILLE EQUATION

In this Appendix the normal solution to the Liouville equation  $\rho_n$  is obtained to first order in the gradients. First write it as a deviation from the local HCS defined in Appendix D

$$\rho = \rho_{h\ell} + \Delta. \quad (\text{E1})$$

Substitution into the Liouville equation gives (7.3)

$$\partial_t \Delta + \int d\mathbf{r} \frac{\delta \Delta}{\delta y_\alpha(\mathbf{r}, t)} N_\alpha(\mathbf{r}, t \mid \{y_\alpha(t)\}) + \bar{L} \Delta = - \int d\mathbf{r} \frac{\delta \rho_{h\ell}}{\delta y_\alpha(\mathbf{r}, t)} N_\alpha(\mathbf{r}, t \mid \{y_\alpha(t)\}) - \bar{L} \rho_{h\ell}. \quad (\text{E2})$$

where the time derivative is taken at constant  $\{y_\beta\}$ . The assumption is that  $\rho_{h\ell}$  has been chosen as the correct reference state in order that  $\Delta$  is of first order in the gradients. This requires that the right side of (5.8) should be proportional to the gradients. To show this, represent  $\rho_{h\ell}$  as an expansion to first order in the gradients about the reference values  $\{y_\alpha(\mathbf{r}, t)\}$

$$\begin{aligned} \rho_{h\ell} &= \rho_h(\{y_\alpha(\mathbf{r}, t)\}) + \int d\mathbf{r}' \left( \frac{\delta \rho_{h\ell}}{\delta y_\beta(\mathbf{r}', t)} \right)_{\delta y=0} (y_\beta(\mathbf{r}', t) - y_\beta(\mathbf{r}, t)) + \dots \\ &= \rho_h(\{y_\alpha(\mathbf{r}, t)\}) + \mathbf{m}_\beta(\mathbf{r}, \{y_\alpha(\mathbf{r}, t)\}) \cdot \nabla y_\beta(\mathbf{r}, t) + \dots \end{aligned} \quad (\text{E3})$$

where the dots denote terms of higher order in the gradients, and  $\mathbf{m}_\nu$  is defined by

$$\begin{aligned} \mathbf{m}_\nu(\mathbf{r}, \{y_\alpha(\mathbf{r}, t)\}) &\equiv \int d\mathbf{r}'' \left( \frac{\delta \rho_{h\ell}}{\delta y_\nu(\mathbf{r}'', t)} \right)_{\delta y=0} (\mathbf{r}'' - \mathbf{r}) \\ &\equiv \mathbf{M}_\nu(\{y_\alpha(\mathbf{r}, t)\}) - \mathbf{r} \frac{\partial \rho_h(\{y_\alpha(\mathbf{r}, t)\})}{\partial y_\alpha(\mathbf{r}, t)} \end{aligned} \quad (\text{E4})$$

With this expansion for  $\rho_{h\ell}$  the functional derivative on the right side can be evaluated

$$\begin{aligned} &\int d\mathbf{r}' \frac{\delta \rho_{h\ell}}{\delta y_\alpha(\mathbf{r}', t)} N_\alpha(\mathbf{r}', t \mid \{y_\alpha\}) = \frac{\partial \rho_h(\{y_\alpha(\mathbf{r}, t)\})}{\partial y_\alpha(\mathbf{r}, t)} N_\alpha(\mathbf{r}, t \mid \{y_\alpha\}) \\ &+ \frac{\partial \mathbf{m}_\beta(\mathbf{r}, \{y_\alpha(\mathbf{r}, t)\})}{\partial y_\alpha(\mathbf{r}, t)} N_\alpha(\mathbf{r}, t \mid \{y_\alpha\}) \cdot \nabla y_\beta(\mathbf{r}, t) \\ &+ \mathbf{m}_\alpha(\mathbf{r}, \{y_\alpha(\mathbf{r}, t)\}) \cdot \nabla N_\alpha(\mathbf{r}, t \mid \{y_\alpha\}) \end{aligned} \quad (\text{E5})$$

The last two terms are of first order in the gradients so it is sufficient to use the lowest order

form  $N_\alpha(\mathbf{r}, t \mid \{y_\alpha\}) \rightarrow -\delta_{\alpha 2} \zeta_h(\{y_\alpha(\mathbf{r}, t)\}) T(\mathbf{r}, t)$  to get

$$\begin{aligned} \int d\mathbf{r}' \frac{\delta \rho_{h\ell}}{\delta y_\alpha(\mathbf{r}', t)} N_\alpha(\mathbf{r}', t \mid \{y_\alpha\}) &= \frac{\partial \rho_h(\{y_\alpha(\mathbf{r}, t)\})}{\partial y_\alpha(\mathbf{r}, t)} N_\alpha(\mathbf{r}, t \mid \{y_\alpha\}) \\ &\quad - \zeta_h(\{y_\alpha(\mathbf{r}, t)\}) T(\mathbf{r}, t) \frac{\partial \mathbf{m}_\beta(\mathbf{r}, \{y_\alpha(\mathbf{r}, t)\})}{\partial T(\mathbf{r}, t)} \\ &\quad + \mathbf{m}_2(\mathbf{r}, \{y_\alpha(\mathbf{r}, t)\}) \cdot \frac{\partial \zeta_h(\{y_\alpha(\mathbf{r}, t)\}) T(\mathbf{r}, t)}{\partial y_\beta(\mathbf{r}, t)} \cdot \nabla y_\beta(\mathbf{r}, t) \end{aligned} \quad (\text{E6})$$

The right side of (E2) is now

$$\begin{aligned} - \int d\mathbf{r}' \frac{\delta \rho_{h\ell}}{\delta y_\alpha(\mathbf{r}', t)} N_\alpha(\mathbf{r}', t \mid \{y_\alpha\}) - \bar{L} \rho_{h\ell} &= -\bar{\mathcal{L}}_T \rho_h - (\bar{\mathcal{L}}_T \mathbf{m}_\beta(\mathbf{r}, \{y_\alpha(\mathbf{r}, t)\}) \\ &\quad + \mathbf{m}_2(\mathbf{r}, \{y_\alpha(\mathbf{r}, t)\}) \frac{\partial \zeta_h(\{y_\alpha(\mathbf{r}, t)\}) T(\mathbf{r}, t)}{\partial y_\beta(\mathbf{r}, t)}) \cdot \nabla y_\beta(\mathbf{r}, t) \\ &\quad - \frac{\partial \rho_h(\{y_\alpha(\mathbf{r}, t)\})}{\partial y_\alpha(\mathbf{r}, t)} (N_\alpha(\mathbf{r}, t \mid \{y_\alpha\}) \\ &\quad + \delta_{\alpha 2} \zeta_h(\{y_\alpha(\mathbf{r}, t)\}) T(\mathbf{r}, t)). \end{aligned} \quad (\text{E7})$$

The operator  $\bar{\mathcal{L}}_T$  is the same as that introduced in Section III, except with the HCS values  $\{y_{h\alpha}\}$  replaced by the true values at the point of interest,  $\{y_\alpha(\mathbf{r}, t)\}$

$$\bar{\mathcal{L}}_T X(\{y_\alpha(\mathbf{r}, t)\}) \equiv -\zeta_h(\{y_\alpha(\mathbf{r}, t)\}) T(\mathbf{r}, t) \frac{\partial X(\{y_\alpha(\mathbf{r}, t)\})}{\partial T(\mathbf{r}, t)} + \bar{L} X. \quad (\text{E8})$$

The first term of (E7) vanishes,  $\bar{\mathcal{L}}_T \rho_h = 0$ . This is the first important consequence of the choice  $\rho_{h\ell}$  for the reference state; it is a solution to the Liouville equation to first order in the gradients.

Next consider the last term of (E7) and recall that  $N_\alpha(\mathbf{r}, t \mid \{y_\alpha\})$  arises from averaging the microscopic conservation laws

$$\begin{aligned} N_\alpha(\mathbf{r}, t \mid \{y_\alpha\}) &= \int d\Gamma (L \tilde{a}_\alpha(\mathbf{r}, \{y_\alpha(\mathbf{r}, t)\})) \rho_n = - \int d\Gamma \tilde{a}_\alpha(\mathbf{r}, \{y_\alpha(\mathbf{r}, t)\}) \bar{L} \rho_n \\ &= - \int d\Gamma \tilde{a}_\alpha(\mathbf{r}, \{y_\alpha(\mathbf{r}, t)\}) \left( \bar{\mathcal{L}}_T \rho_n + \zeta_h(\{y_\alpha\}) T \frac{\partial \rho_n}{\partial T} \right) \end{aligned} \quad (\text{E9})$$

where  $\tilde{a}_\alpha(\mathbf{r}, \{y_\alpha(\mathbf{r}, t)\})$  are linear combinations of the local densities of number, energy, and momentum

$$\tilde{a}_\alpha(\mathbf{r}, \{y_\alpha(\mathbf{r}, t)\}) = \begin{pmatrix} \hat{n}(\mathbf{r}) - n(\mathbf{r}, t) \\ \frac{2}{3n(\mathbf{r}, t)} (\hat{\epsilon}'(\mathbf{r}) - \frac{3}{2} T(\mathbf{r}, t) \hat{n}(\mathbf{r})) \\ \frac{1}{n(\mathbf{r}, t)m} \hat{\mathbf{g}}'(\mathbf{r}) \end{pmatrix}. \quad (\text{E10})$$



Note that

$$\begin{aligned}
\int d\Gamma \tilde{a}_\alpha(\mathbf{r}, \{y_\alpha(\mathbf{r}, t)\}) \zeta_h(\{y_\alpha\}) T \frac{\partial \rho_n}{\partial T} &= \zeta_h(\{y_\alpha\}) T \frac{\partial}{\partial T} \int d\Gamma \tilde{a}_\alpha(\mathbf{r}, \{y_\alpha(\mathbf{r}, t)\}) \rho_n \\
&\quad - \zeta_h(\{y_\alpha\}) T \int d\Gamma \frac{\partial \tilde{a}_\alpha(\mathbf{r}, \{y_\alpha(\mathbf{r}, t)\})}{\partial T} \rho_n \\
&= \delta_{\alpha 2} \zeta_h(\{y_\alpha\}) T,
\end{aligned} \tag{E11}$$

so

$$\begin{aligned}
N_\alpha(\mathbf{r}, t \mid \{y_\alpha\}) + \delta_{\alpha 2} \zeta_h(\{y_\alpha\}) T &= - \int d\Gamma \tilde{a}_\alpha(\mathbf{r}, \{y_\alpha(\mathbf{r}, t)\}) \bar{\mathcal{L}}_T (\rho_{h\ell} + \Delta) \\
&= - \int d\Gamma \tilde{a}_\alpha(\mathbf{r}, \{y_\alpha(\mathbf{r}, t)\}) \bar{\mathcal{L}}_T \mathbf{m}_\beta(\mathbf{r}, \{y_\alpha(\mathbf{r}, t)\}) \cdot \nabla y_\beta(\mathbf{r}, t) \\
&\quad - \int d\Gamma \tilde{a}_\alpha(\mathbf{r}, \{y_\alpha(\mathbf{r}, t)\}) \bar{\mathcal{L}}_T \Delta
\end{aligned} \tag{E12}$$

With these results the Liouville equation (E2) becomes

$$\begin{aligned}
\partial_t \Delta + \int d\mathbf{r} \frac{\delta \Delta}{\delta y_\alpha(\mathbf{r}, t)} N_\alpha(\mathbf{r}, t \mid \{y_\alpha\}) + \bar{L} \Delta - \frac{\partial \rho_h(\{y_\alpha(\mathbf{r}, t)\})}{\partial y_\alpha(\mathbf{r}, t)} \int d\Gamma \tilde{a}_\alpha(\mathbf{r}, \{y_\alpha(\mathbf{r}, t)\}) \bar{\mathcal{L}}_T \Delta \\
= - \left( \bar{\mathcal{L}}_T \mathbf{m}_\beta(\mathbf{r}, \{y_\alpha(\mathbf{r}, t)\}) + \mathbf{m}_2(\mathbf{r}, \{y_\alpha(\mathbf{r}, t)\}) \frac{\partial \zeta_h(\{y_\alpha(\mathbf{r}, t)\}) T(\mathbf{r}, t)}{\partial y_\beta(\mathbf{r}, t)} \right) \cdot \nabla y_\beta(\mathbf{r}, t) \\
+ \frac{\partial \rho_h(\{y_\alpha(\mathbf{r}, t)\})}{\partial y_\alpha(\mathbf{r}, t)} \int d\Gamma \tilde{a}_\alpha(\mathbf{r}, \{y_\alpha(\mathbf{r}, t)\}) \bar{\mathcal{L}}_T \mathbf{m}_\beta(\mathbf{r}, \{y_\alpha(\mathbf{r}, t)\}) \cdot \nabla y_\beta(\mathbf{r}, t)
\end{aligned} \tag{E13}$$

The right side is now explicitly proportional to the gradients, so a solution of the form (6.1) is possible

$$\Delta = \int d\mathbf{r} \mathbf{G}_\alpha(\Gamma, \mathbf{r}, t \mid \{y_\alpha(\mathbf{r}, t)\}) \cdot \nabla y_\alpha(\mathbf{r}, t). \tag{E14}$$

This is a direct consequence of the choice of  $\rho_{h\ell}$  as the reference state, as seen by the above analysis where all terms of zeroth order in the gradients cancel. Substitution of (E14) into (E13), evaluating the functional derivatives on the left side, and equating coefficients of the gradients gives the desired equation for  $\mathbf{G}_\alpha(\Gamma, \mathbf{r}, t \mid \{y_\alpha\})$  (here and below it is understood that all fields are evaluated at  $y_\alpha = y_\alpha(\mathbf{r}, t)$ )

$$\begin{aligned}
\partial_t \Delta + \left( \bar{\mathcal{L}}_T \mathbf{G}_\beta(t, \{y_\alpha\}) + \mathbf{G}_2(t, \{y_\alpha\}) \frac{\partial \zeta_h(\{y_\alpha\}) T}{\partial y_\beta} \right) \\
- \frac{\partial \rho_h(\{y_\alpha\})}{\partial y_\alpha} \int d\Gamma \tilde{a}_\alpha(\mathbf{r}, \{y_\alpha\}) \bar{\mathcal{L}}_T \mathbf{G}_\beta(t, \{y_\alpha\}) \\
= - \left( \bar{\mathcal{L}}_T \mathbf{m}_\beta(\mathbf{r}, \{y_\alpha\}) + \mathbf{m}_2(\mathbf{r}, \{y_\alpha\}) \frac{\partial \zeta_h(\{y_\alpha\}) T}{\partial y_\beta} \right) \\
+ \frac{\partial \rho_h(\{y_\alpha\})}{\partial y_\alpha} \int d\Gamma \tilde{a}_\alpha(\mathbf{r}, \{y_\alpha\}) \bar{\mathcal{L}}_T \mathbf{m}_\beta(\mathbf{r}, \{y_\alpha\})
\end{aligned} \tag{E15}$$

The structure of this equation can be exposed further by introducing a set of functions  $\{\psi_\alpha\}$  that are biorthogonal to the set  $\{\tilde{a}_\alpha\}$

$$\psi_\alpha(\mathbf{r}', \{y_\alpha\}) = \left( \frac{\delta \rho_{h\ell}(\{y_\alpha\})}{\delta y_\alpha(\mathbf{r}', t)} \right)_{\delta y=0}. \quad (\text{E16})$$

The biorthogonality property is

$$\begin{aligned} \int d\Gamma \tilde{a}_\alpha(\mathbf{r}, \{y_\alpha\}) \psi_\beta(\mathbf{r}', \{y_\alpha\}) &= \left( \frac{\delta}{\delta y_\beta(\mathbf{r}', t)} \int d\Gamma \tilde{a}_\alpha(\mathbf{r}, \{y_\alpha\}) \rho_{h\ell}(\{y_\alpha\}) \right)_{\delta y=0} \\ &\quad - \int d\Gamma \frac{\delta \tilde{a}_\alpha(\mathbf{r}, \{y_\alpha\})}{\delta y_\beta(\mathbf{r}', t)} \rho_h(\{y_\alpha\}) \\ &= \delta(\mathbf{r}' - \mathbf{r}) \delta_{\alpha\beta} \end{aligned} \quad (\text{E17})$$

Integrating over  $\mathbf{r}'$  gives the related orthogonality condition

$$\frac{1}{V} \int d\Gamma \tilde{A}_\beta \Psi_\alpha = \delta_{\alpha\beta}, \quad (\text{E18})$$

where

$$\Psi_\alpha(\{y_\alpha\}) = \frac{\partial \rho_h(\{y_\alpha\})}{\partial y_\alpha}, \quad \tilde{A}_\beta(\{y_\alpha\}) = \int d\mathbf{r} \begin{pmatrix} \hat{N} - N \\ \frac{2}{3n} \left( \hat{H}' - \frac{3}{2} T \hat{N} \right) \\ \frac{1}{nm} \hat{\mathbf{P}}' \end{pmatrix}. \quad (\text{E19})$$

Several useful identities follow from the condition that the averages of fields  $\tilde{a}_\alpha(\mathbf{r}, \{y_\alpha\})$  vanish for  $\rho_{h\ell}$  and therefore, according to (6.2)

$$\int d\Gamma \tilde{a}_\alpha(\mathbf{r}, \{y_\alpha(\mathbf{r}, t)\}) \rho_{h\ell}(\{y_\alpha(\mathbf{r}, t)\}) = 0 = \int d\Gamma \tilde{A}_\alpha(\{y_\alpha(\mathbf{r}, t)\}) \rho_{h\ell}(\{y_\alpha(\mathbf{r}, t)\}). \quad (\text{E20})$$

Direct calculation gives the same result for  $\rho_h(\{y_\alpha\})$

$$\int d\Gamma \tilde{a}_\alpha(\mathbf{r}, \{y_\alpha(\mathbf{r}, t)\}) \rho_h(\{y_\alpha\}) = 0 = \int d\Gamma \tilde{A}_\alpha(\{y_\alpha(\mathbf{r}, t)\}) \rho_h(\{y_\alpha(\mathbf{r}, t)\}). \quad (\text{E21})$$

This implies

$$\int d\Gamma \tilde{a}_\alpha(\mathbf{r}, \{y_\alpha(\mathbf{r}, t)\}) \mathbf{m}_\beta(\mathbf{r}, \{y_\alpha(\mathbf{r}, t)\}) = 0 = \int d\Gamma \tilde{A}_\alpha(\{y_\alpha(\mathbf{r}, t)\}) \mathbf{m}_\beta(\mathbf{r}, \{y_\alpha(\mathbf{r}, t)\}) \quad (\text{E22})$$

$$\int d\Gamma \tilde{a}_\alpha(\mathbf{r}, \{y_\alpha(\mathbf{r}, t)\}) \mathbf{G}_\beta(t, \{y_\alpha(\mathbf{r}, t)\}) = 0 = \int d\Gamma \tilde{A}_\alpha(\{y_\alpha(\mathbf{r}, t)\}) \mathbf{G}_\beta(t, \{y_\alpha(\mathbf{r}, t)\}) \quad (\text{E23})$$

Finally, define the projection operator  $\mathcal{P}$  by

$$\mathcal{P}X = \Psi_\alpha \frac{1}{V} \int d\Gamma \tilde{A}_\alpha X. \quad (\text{E24})$$

Then (E15) takes the final form

$$(\partial_t + (1 - \mathcal{P}) (I\bar{\mathcal{L}}_T + K^T)) \mathbf{G}(t, \{y_\alpha\}) = - (1 - \mathcal{P}) (I\bar{\mathcal{L}}_T + K^T) \mathbf{M}(\{y_\alpha\}) \quad (\text{E25})$$

Here  $I$  is the unit matrix and  $K^T$  is the transpose of the matrix

$$K = \begin{pmatrix} 0 & 0 & 0 \\ \frac{\partial(\zeta_h T)}{\partial n} & \frac{\partial(\zeta_h T)}{\partial T} & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad (\text{E26})$$

The matrix  $K$  generates the solution to the hydrodynamic equations in the absence of gradients, Eqs. (6.18).

The explicit dependence on  $\mathbf{r}$  has cancelled in (E25) (as it must, for a normal solution) as a consequence of

$$(I\bar{\mathcal{L}}_T + K^T) \mathbf{r} \Psi = \mathbf{r} (I\bar{\mathcal{L}}_T + K^T) \Psi = 0. \quad (\text{E27})$$

The second equality follows from the fact that  $\Psi$  form the null space for  $(I\bar{\mathcal{L}}_T + K^T)$

$$(I\bar{\mathcal{L}}_T + K^T) \Psi = 0. \quad (\text{E28})$$

This can be demonstrated by direct calculation

$$\begin{aligned} (I\bar{\mathcal{L}}_T + K^T)_{\alpha\beta} \Psi_\beta &= (\bar{L}\Psi_\alpha - \zeta_h T \partial_T + K_{\alpha 2}^T \Psi_2) \\ &= \frac{\partial \bar{L} \rho_h}{\partial y_\alpha} - \zeta_h T \frac{\partial \Psi_2}{\partial y_\alpha} + K_{\alpha 2}^T \Psi_2 \\ &= \frac{\partial \zeta_h T \Psi_2}{\partial y_\alpha} - \zeta_h T \frac{\partial \Psi_2}{\partial y_\alpha} + K_{\alpha 2}^T \Psi_2 = 0 \end{aligned} \quad (\text{E29})$$

Equation (E25) is the primary result of this Appendix, giving the exact solution to the Liouville equation up to first order in the gradients. As a final simplification, a transformation from the operator  $\bar{\mathcal{L}}_T$  to the phase space operator  $\bar{\mathcal{L}}$  of (3.27) can be made by introducing dimensionless variables

$$\begin{aligned} \mathbf{G}_1(\Gamma, t, \{y_\alpha\}) &= \frac{\ell}{n} (\ell v(T))^{-3N} \mathbf{G}_1^*(\Gamma^*, s, n\ell^3), \\ \mathbf{G}_2(\Gamma, t, \{y_\alpha\}) &= \frac{\ell}{T} (\ell v(T))^{-3N} \mathbf{G}_2^*(\Gamma^*, s, n\ell^3), \\ \mathbf{G}_3(\Gamma, t, \{y_\alpha\}) &= \frac{\ell}{T^{1/2}} (\ell v(T))^{-3N} \mathbf{G}_2^*(\Gamma^*, s, n\ell^3) \end{aligned} \quad (\text{E30})$$

The first factor in each case gives the dimensions to compensate for the associate gradient multiplying  $\mathbf{G}_\alpha$ . The second time arises in each case because the solution to the

Liouville equation is a density in phase space. The dimensionless phase point  $\Gamma^* \equiv \{\mathbf{q}_1^*, \dots, \mathbf{q}_N^*, \mathbf{V}_1^*, \dots, \mathbf{V}_N^*\}$  is defined by

$$\mathbf{q}_r^* = \mathbf{q}_r / \ell, \quad \mathbf{V}_r^* = (\mathbf{v}_r - \mathbf{U}(\mathbf{r}, t)) / v_h(t) \quad (\text{E31})$$

where  $v_h(t)$  is the thermal velocity defined in (3.22), with  $T_h \rightarrow T(\mathbf{r}, t)$ . With these definitions

$$\begin{aligned} (\partial_t |_{\Gamma, \{y_\alpha\}} - \zeta_h T \partial_T |_{\Gamma, t}) &= \frac{v_h(t)}{\ell} \left( \frac{\ell}{v_h(t)} \partial_t |_{\Gamma^*, \{y_\alpha\}} - \zeta_h^* T \partial_T |_{\Gamma^*, t} + \frac{\zeta_h^*}{2} \sum_{r=1}^N (3 + \mathbf{V}_r^* \cdot \nabla_{\mathbf{V}_r^*}) \right) \\ &= \frac{v_h(t)}{\ell} \left( \frac{\ell}{v_h(t)} \partial_t |_{\Gamma^*, \{y_\alpha\}} - \zeta_h^* T \frac{\partial s}{\partial T} |_t \partial_s |_{\Gamma^*} \right. \\ &\quad \left. - \zeta_h^* T \partial_T |_{\Gamma^*, s} + \frac{\zeta_h^*}{2} \sum_{r=1}^N (3 + \mathbf{V}_r^* \cdot \nabla_{\mathbf{V}_r^*}) \right) \end{aligned} \quad (\text{E32})$$

Here  $s = s(t, T)$  is a dimensionless time scale, and  $\zeta_h^*$  is the constant dimensionless cooling rate of (3.31). A judicious choice for the dimensionless time is seen to be

$$\frac{\ell}{v_h(t)} \partial_t |_{\Gamma, \{y_\alpha\}} - \zeta_h^* T \frac{\partial s}{\partial T} |_t \partial_s |_{\Gamma^*} \equiv \partial_s |_{\Gamma^*} \quad (\text{E33})$$

or

$$\frac{ds}{(1 + \zeta_h^* T \frac{\partial s}{\partial T} |_t)} \equiv \frac{v_h(t)}{\ell} dt. \quad (\text{E34})$$

It can be shown that this definition agrees with that of (3.35) in the sense  $s(t) = s(t, T(t))$

$$ds(t) = \frac{v_h(T(t))}{\ell} dt, \quad T(t) = T(0) \left( 1 + \frac{v_h(0) \zeta_h^*}{2\ell} t \right)^{-2}. \quad (\text{E35})$$

Equation (E32) simplifies to

$$(\partial_t |_{\Gamma, \{y_\alpha\}} - \zeta_h T \partial_T |_{\Gamma, t}) = \frac{v_h(t)}{\ell} \left( \partial_s |_{\Gamma^*} - \zeta_h^* T \partial_T |_{\Gamma^*, s} + \frac{\zeta_h^*}{2} \sum_{r=1}^N (3 + \mathbf{V}_r^* \cdot \nabla_{\mathbf{V}_r^*}) \right). \quad (\text{E36})$$

Now, taking into account the forms (E30), the equation (E25) for  $\mathbf{G}_\alpha$  has the corresponding dimensionless form

$$\left( \partial_s + (1 - \mathcal{P}^*) \left( I \bar{\mathcal{L}}^* - \bar{\Lambda}^* + K^{T*} \right) \right) \mathbf{G}^* = - (1 - \mathcal{P}^*) \left( I \bar{\mathcal{L}}^* - \bar{\Lambda}^* + K^{T*} \right) \mathbf{M}^* (\{y_\alpha\}), \quad (\text{E37})$$

where an asterisk denotes the function, operator, or matrix in terms of the dimensionless variables. The matrix  $\bar{\Lambda}^*$  arises from the first factors of (E30) associated with the dimensions

of the respective gradients.

$$\overline{\Lambda}^* = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \zeta_h^* & 0 \\ 0 & 0 & \frac{1}{2}\zeta_h^* \end{pmatrix}. \quad (\text{E38})$$

The notation is simplified by introducing the matrix  $\Lambda^*$

$$\Lambda^* = K^{T*} - \overline{\Lambda}^* = \begin{pmatrix} 0 & \frac{\partial(\zeta_h T)}{Tv_h \ell^2 \partial n} & 0 \\ 0 & \frac{1}{2}\zeta_h^* & 0 \\ 0 & 0 & -\frac{1}{2}\zeta_h^* \end{pmatrix}. \quad (\text{E39})$$

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